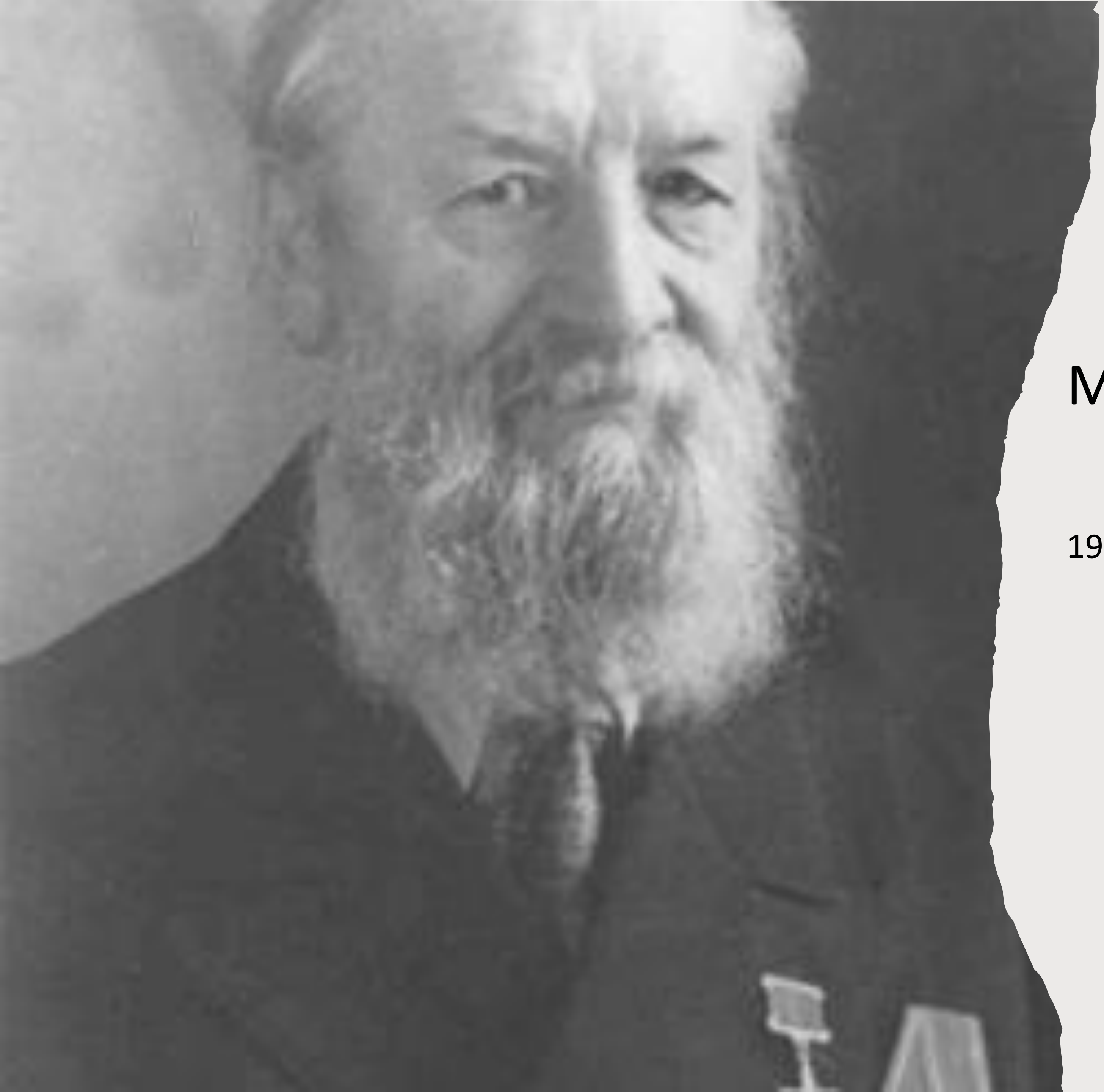
Clase # 4:

Dinámica cuántica en el subespacio de Krylov: métodos y aplicaciones

Diego A. Wisniacki, UBA



Método del subespacio de Krylov

1931 método para calcular autovalores de una matriz

A. Krylov fue un ingeniero naval y matemático aplicado ruso

Usando el método de Krylov en evoluciones cuánticas

Problem that I want to solve

$|\psi\rangle$ Initial state

$\mathcal{H} = \mathbb{C}^D$ H Hamiltonian

We want to find $|\psi(t)\rangle = e^{-iHt}|\psi\rangle$

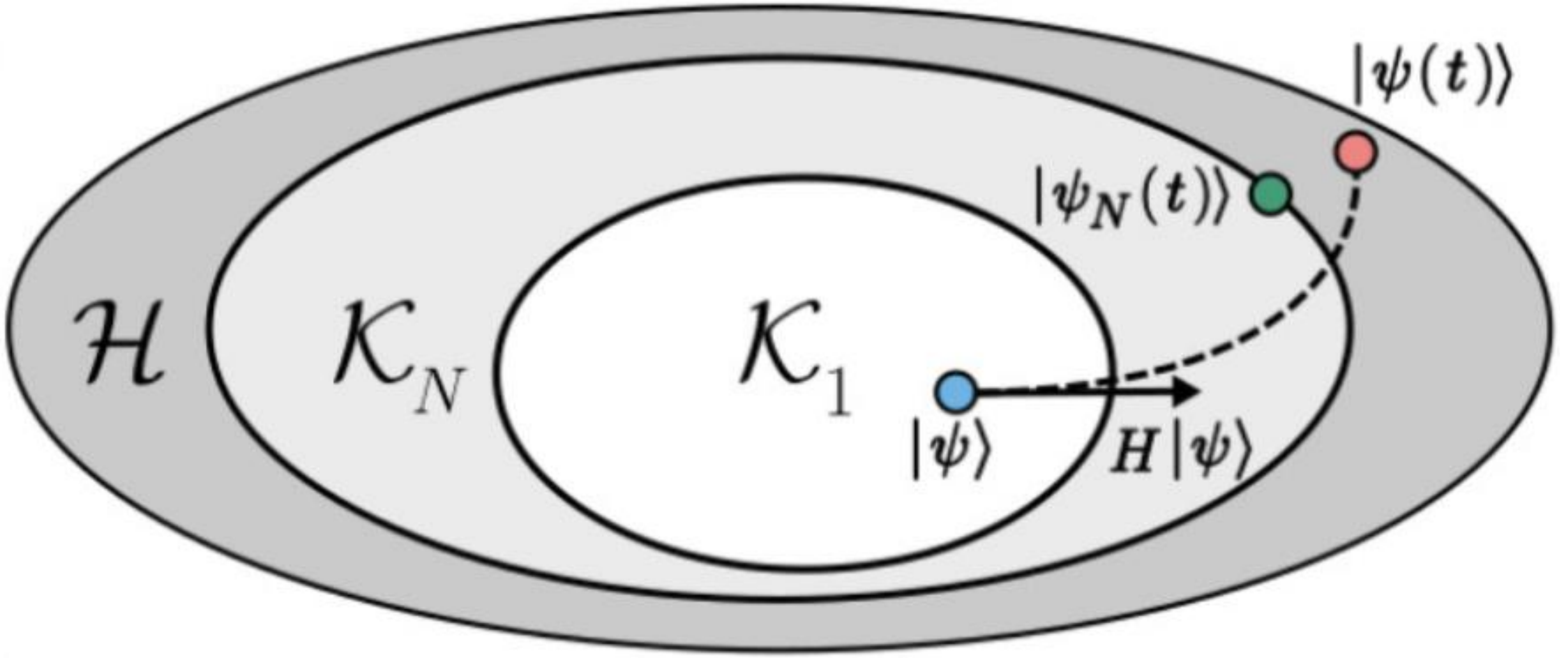
$$|\psi(t)\rangle_{ap} = e^{-iHt}{}_{ap}|\psi\rangle$$

$$|\langle\psi(t)|\psi(t)\rangle_{ap}|^2 \leq \epsilon.$$

El desafío central en los métodos de subespacio de Krylov es mantener el error en valores bajos y, por lo tanto, lograr una evolución precisa.

Krylov method

$$\mathcal{K}_N = \text{span}\{|\psi\rangle, H|\psi\rangle, \dots, H^{N-1}|\psi\rangle\}$$



The Krylov approach aims at approximating the time-evolved state $|\psi(t)\rangle$ with the best element $|\psi_N(t)\rangle \in \mathcal{K}_N$.

To do so, we first have to build an orthonormal basis for K_N

$$\{|v_0\rangle \equiv |\psi\rangle, \ldots, |v_{N-1}\rangle\}$$

Algorithm1 Lanczos Algorithm. Receives state $|\psi\rangle$ and Hamiltonian H and returns a set of N orthonormal vectors $\{|v_i\rangle\}$ spanning the Krylov subspace $\mathcal{K}_N$.

$|v_0\rangle = |\psi\rangle$ (assume normalized)
$|x_1\rangle = H|\psi\rangle$
$\alpha_1 = \langle x_1|v_0\rangle$ (the component of $|x_1\rangle$ in $|v_0\rangle$)
$|w_1\rangle = |x_1\rangle - \alpha_1|v_0\rangle$
for $j = 1, 2, \ldots$ **do**
    $\beta_j = \sqrt{\langle\omega_j|\omega_j\rangle}$
    if $\beta_j > 0$ **then**
        $|v_j\rangle \leftarrow \frac{1}{\beta_j}|\omega_j\rangle$.
    else
        break
    $|x_{j+1}\rangle = H|v_j\rangle$
    $\alpha_{j+1} = \langle x_{j+1}|v_j\rangle$
    $|\omega_{j+1}\rangle = |x_{j+1}\rangle - \alpha_{j+1}|v_j\rangle - \beta_j|v_{j-1}\rangle$

$$|\psi(t)\rangle = e^{-iHt}\,|\psi\rangle \approx \mathbb{P}_N e^{-iHt}\mathbb{P}_N\,|\psi\rangle$$

$$\mathbb{P}_N = \sum_{i=0,N-1} |v_i\rangle\,\langle v_i|$$

$$\mathbb{V}_N^\dagger = \begin{bmatrix} \vdots & \vdots & & \vdots \\ |v_0\rangle\,, & |v_1\rangle\,, & & ,|v_{N-1}\rangle \\ \vdots & \vdots & & \vdots \end{bmatrix} \quad \Rightarrow \quad \mathbb{P}_N = \mathbb{V}_N^\dagger \mathbb{V}_N$$

$$
\begin{aligned}
|\psi(t)\rangle = e^{-iHt}|\psi\rangle &\approx \mathbb{P}_N e^{-iHt}\mathbb{P}_N|\psi\rangle \\
&= \mathbb{V}_N^\dagger e^{-iT_N t}\mathbb{V}_N|\psi\rangle \\
&\equiv |\psi_N(t)\rangle .
\end{aligned}
$$

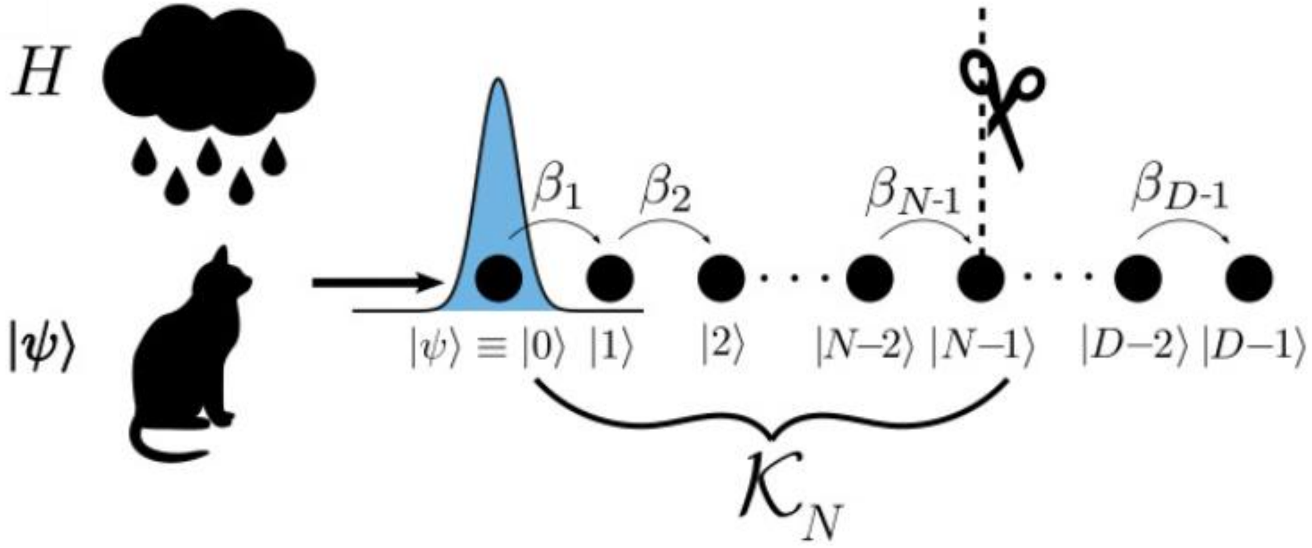
$$
T_N = \mathbb{V}_N H \mathbb{V}_N^\dagger
$$

$$
T_N = \begin{pmatrix}
\alpha_1 & \beta_1 & 0 & \cdots & 0 \\
\beta_1 & \alpha_2 & \beta_2 & \cdots & 0 \\
0 & \beta_2 & \alpha_3 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & \alpha_N
\end{pmatrix}
$$

By definition, V_N maps given initial state into the first coordinate vector of an effective N-dimensional system.

$$\mathbb{V}_N \left|\psi\right\rangle = (1, 0, \cdots, 0)^T \equiv \left|0\right\rangle_N$$

Un estado inicial localizado en un extremo de una cadena efectiva evoluciona de acuerdo a T_N (es decir, con un potencial en el sitio αi y una amplitud de salto βi en el sitio i), propagando la excitación y poblando el resto. Finalmente, $V_N^\dagger$ mapea el estado evolucionado en el espacio efectivo de vuelta al espacio de Hilbert completo. La eficiencia del método radica en el hecho de que la evolución temporal se resuelve con un costo computacional muy bajo en el espacio reducido, es decir, se reemplaza la exponencial de una matriz hermítica H de dimensión $D \times D$ por la mucho más económica exponencial de una matriz tridiagonal simétrica T_N de dimensión $N \times N$. Por supuesto, se asume que $N \ll D$.



H
$|\psi\rangle$
β_1
β_2
$\beta_{N\text{-}1}$
$\beta_{D\text{-}1}$
$|\psi\rangle \equiv |0\rangle$
$|1\rangle$
$|2\rangle$
$|N-2\rangle$
$|N-1\rangle$
$|D-2\rangle$
$|D-1\rangle$
$\mathcal{K}_N$

Usando el eco de Loschmidt para acotar el error en la evolución cuántica por método del subespacio de Krylov

Problem that I want to solve

$|\psi\rangle$ Initial state

$\mathcal{H} = \mathbb{C}^D$ $\quad H$ Hamiltonian

We want to find $|\psi(t)\rangle = e^{-iHt}|\psi\rangle$

$$|\psi(t)\rangle_{ap} = {e^{-iHt}}_{ap}|\psi\rangle$$

$$|\langle\psi(t)|\psi(t)\rangle_{ap}|^2 \leq \epsilon.$$

The core challenge in Krylov-subspace methods is to keep the error at low values and, thus, achieve a precise evolution.

Error in the Krylov-subspace method and the Loschmidt echo

$$\epsilon_N(t) = 1 - |\langle\psi_N(t)|\psi(t)\rangle|^2$$

$$|\langle\psi_N(t)|\psi(t)\rangle|^2 = \left|\langle\psi|\,\mathbb{V}_N^{\dagger}e^{iT_N t}\mathbb{V}_N e^{-iHt}\,|\psi\rangle\right|^2$$

$$\left| \left\langle \psi_N\left(t\right) | \psi\left(t\right) \right\rangle \right|^2 = \left| \left\langle \psi \right| \mathbb{V}_N^\dagger e^{iT_N t} \mathbb{V}_N e^{-iHt} \left| \psi \right\rangle \right|^2$$

$$
\begin{aligned}
\left| \left\langle \psi_N(t) \middle| \psi(t) \right\rangle \right|^2 &= \left| \left\langle \psi \right| \mathbb{V}_N^\dagger e^{iT_N t} \mathbb{V}_N e^{-iHt} \left| \psi \right\rangle \right|^2 \\
&= \left| \left\langle \psi \right| \mathbb{V}_N^\dagger e^{iT_N t} \mathbb{V}_N \mathbb{V}_D^\dagger e^{-iT_D t} \mathbb{V}_D \left| \psi \right\rangle \right|^2
\end{aligned}
$$

$$
\begin{aligned}
|\langle\psi_N(t)|\psi(t)\rangle|^2 &= \left|\langle\psi|\,\mathbb{V}_N^\dagger e^{iT_N t}\mathbb{V}_N e^{-iHt}\,|\psi\rangle\right|^2 \\
&= \left|\langle\psi|\,\mathbb{V}_N^\dagger e^{iT_N t}\mathbb{V}_N \mathbb{V}_D^\dagger e^{-iT_D t}\mathbb{V}_D\,|\psi\rangle\right|^2 \\
&= \left|\langle\psi|\,\mathbb{V}_D^\dagger e^{i\tilde{T}_N t}\mathbb{V}_D \mathbb{V}_D^\dagger e^{-iT_D t}\mathbb{V}_D\,|\psi\rangle\right|^2
\end{aligned}
$$

$$
\begin{aligned}
\left| \left\langle \psi_N\left(t\right) \middle| \psi\left(t\right) \right\rangle \right|^2 &= \left| \left\langle \psi \right| \mathbb{V}_N^\dagger e^{iT_N t} \mathbb{V}_N e^{-iHt} \left| \psi \right\rangle \right|^2 \\
&= \left| \left\langle \psi \right| \mathbb{V}_N^\dagger e^{iT_N t} \mathbb{V}_N \mathbb{V}_D^\dagger e^{-iT_D t} \mathbb{V}_D \left| \psi \right\rangle \right|^2 \\
&= \left| \left\langle \psi \right| \mathbb{V}_D^\dagger e^{i\tilde{T}_N t} \mathbb{V}_D \mathbb{V}_D^\dagger e^{-iT_D t} \mathbb{V}_D \left| \psi \right\rangle \right|^2 \\
&= \left| \left\langle 0 \right| e^{i\tilde{T}_N t} e^{-iT_D t} \left| 0 \right\rangle \right|^2
\end{aligned}
$$

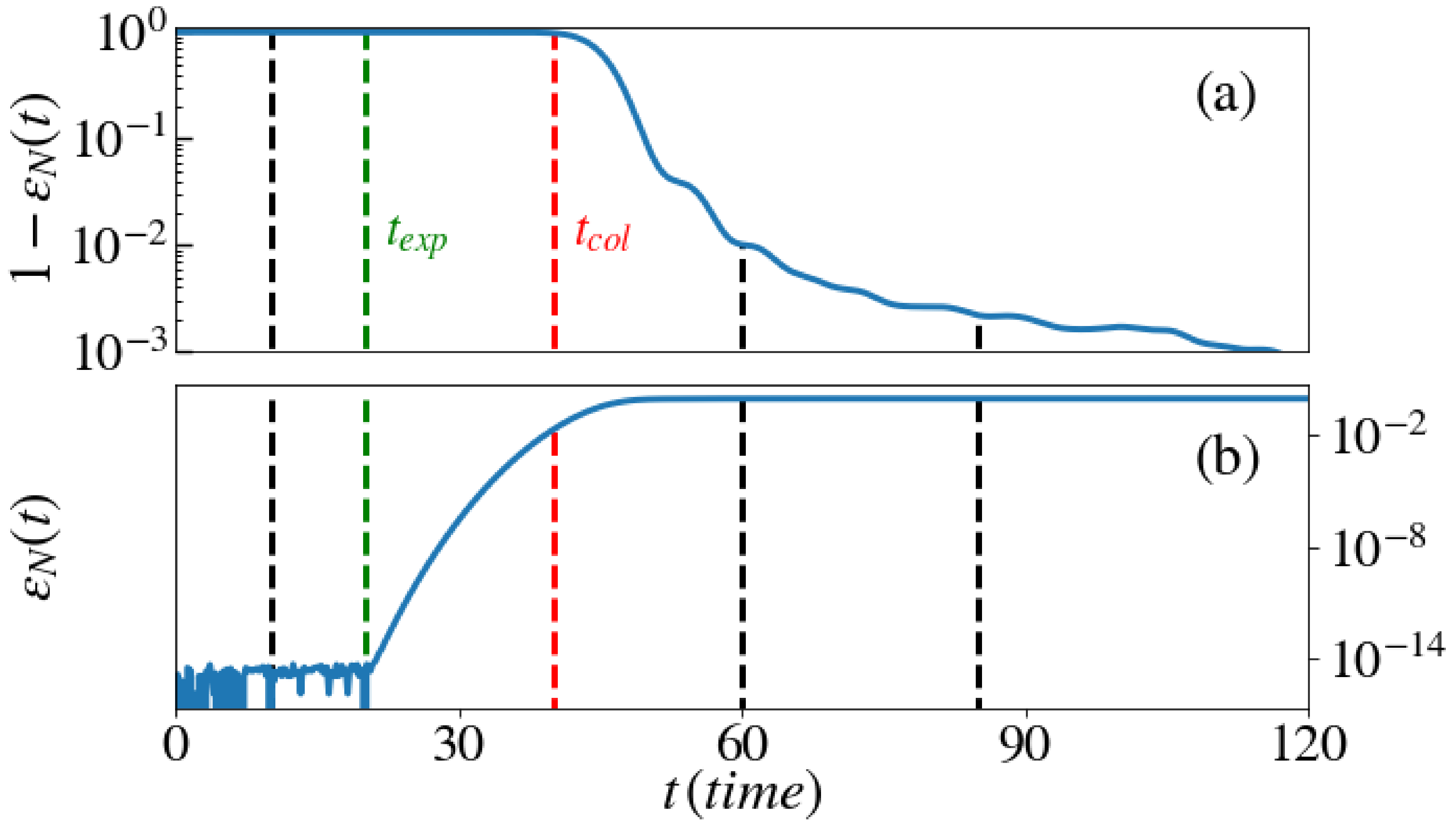
$$
\begin{aligned}
|\langle\psi_N(t)|\psi(t)\rangle|^2 &= \left|\langle\psi|\,\mathbb{V}_N^\dagger e^{iT_N t}\mathbb{V}_N e^{-iHt}\,|\psi\rangle\right|^2 \\
&= \left|\langle\psi|\,\mathbb{V}_N^\dagger e^{iT_N t}\mathbb{V}_N \mathbb{V}_D^\dagger e^{-iT_D t}\mathbb{V}_D\,|\psi\rangle\right|^2 \\
&= \left|\langle\psi|\,\mathbb{V}_D^\dagger e^{i\tilde{T}_N t}\mathbb{V}_D \mathbb{V}_D^\dagger e^{-iT_D t}\mathbb{V}_D\,|\psi\rangle\right|^2 \\
&= \left|\langle 0|\,e^{i\tilde{T}_N t} e^{-iT_D t}\,|0\rangle\right|^2
\end{aligned}
$$

Loschmidt echo!!!!!

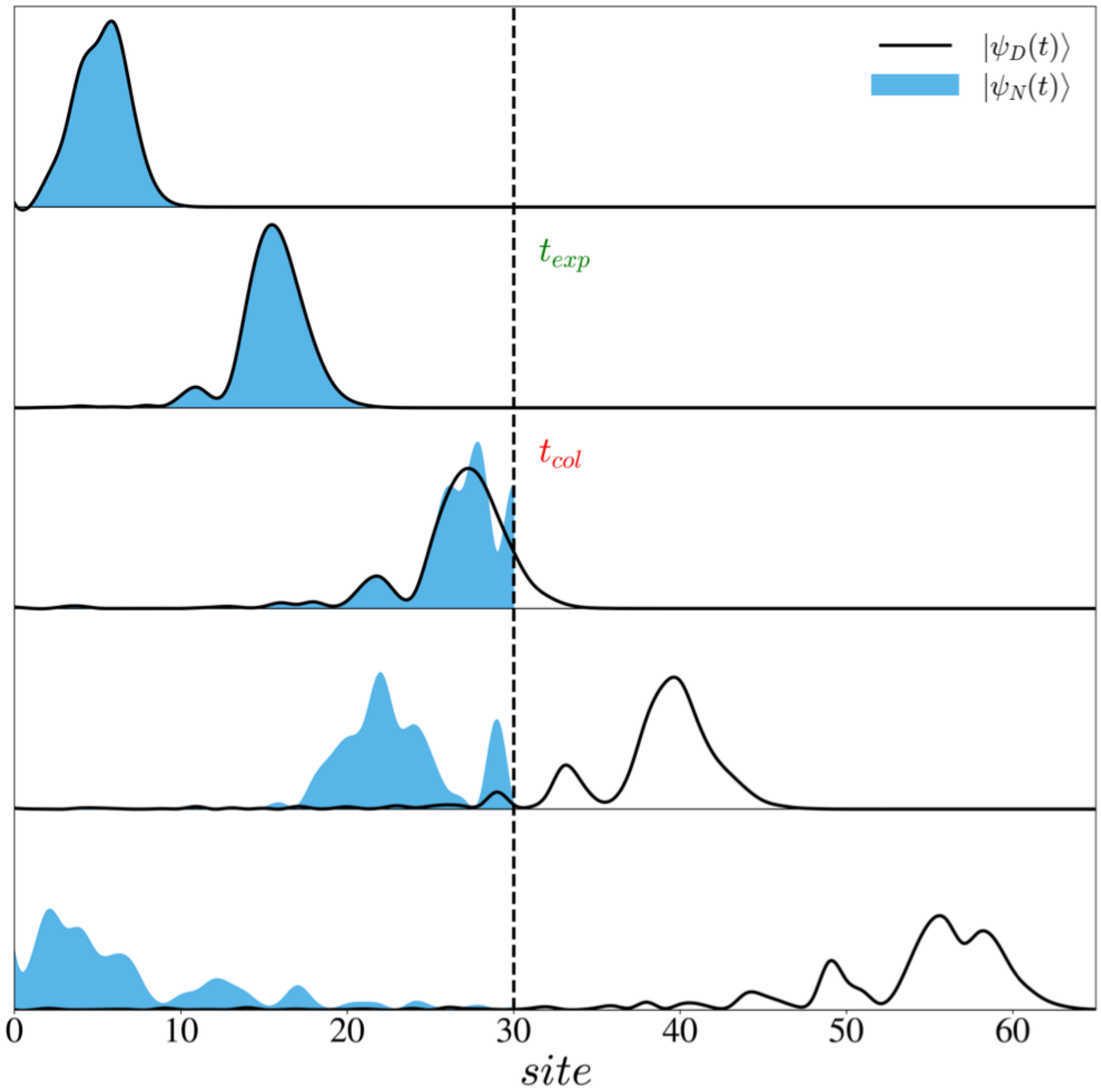
$$
\tilde{T}_N = \left(\begin{array}{c|c} T_N & 0 \\ \hline 0 & 0 \end{array}\right) \qquad \tilde{T}_N = \mathbb{V}_D \mathbb{P}_N H \mathbb{P}_N \mathbb{V}_D^\dagger
$$

Let us see the behaviour of the error

$$H = \sum_{k=1}^{L} (h_x \hat{\sigma}_k^x + h_z \hat{\sigma}_k^z) - J \sum_{k=1}^{L-1} \hat{\sigma}_k^z \hat{\sigma}_{k+1}^z$$



10^0
10^{-1}
10^{-2}
10^{-3}
$1-\varepsilon_N(t)$
(a)
t_{exp}
t_{col}
$\varepsilon_N(t)$
(b)
10^{-2}
10^{-8}
10^{-14}
0
30
60
90
120
$t\,(time)$



$|\psi_D(t)\rangle$
$|\psi_N(t)\rangle$
t_{exp}
t_{col}
0
10
20
30
40
50
60
site

Is generic the that behaviour of the error?

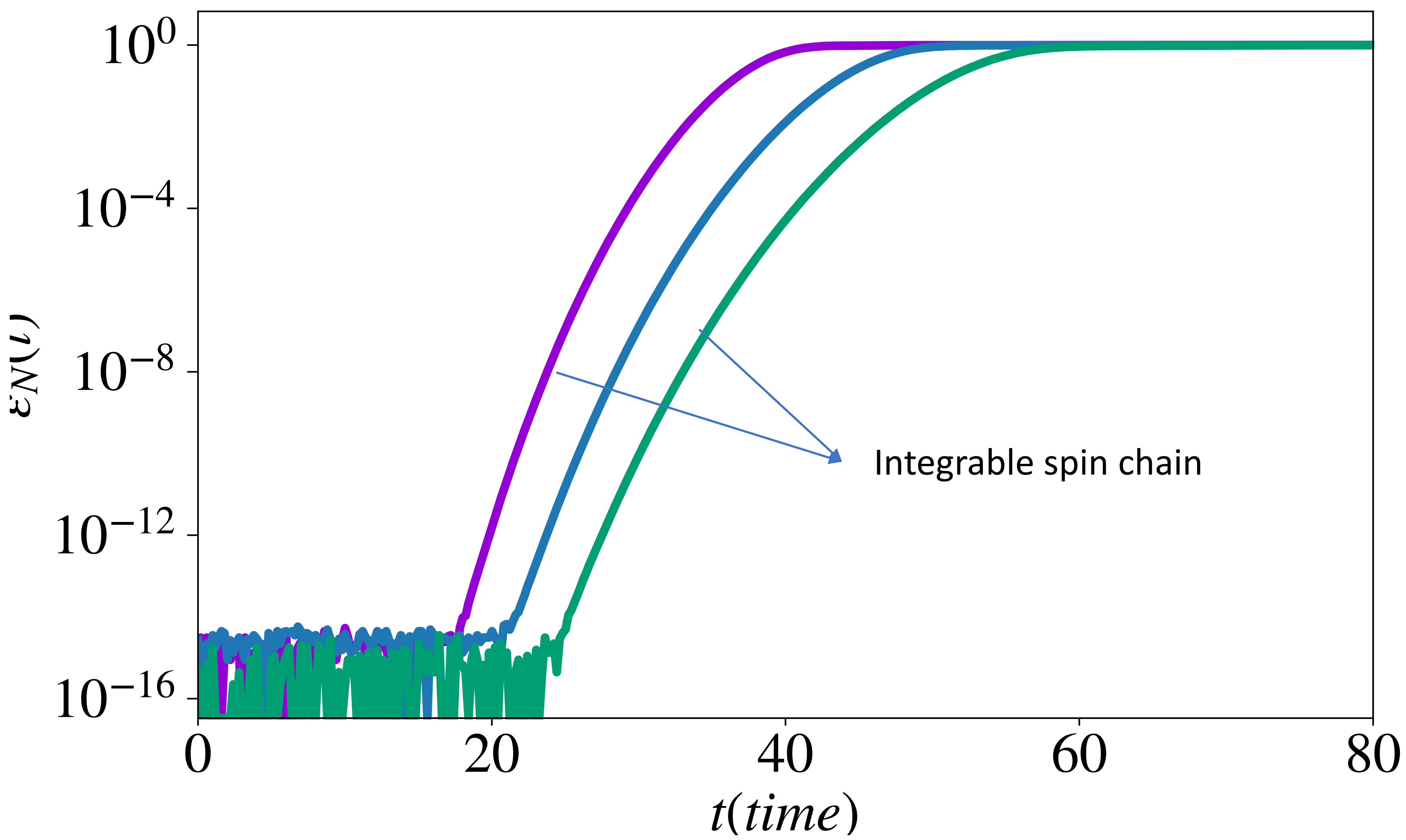
$$H = \sum_{k=1}^{L} (h_x \hat{\sigma}_k^x + h_z \hat{\sigma}_k^z) - J \sum_{k=1}^{L-1} \hat{\sigma}_k^z \hat{\sigma}_{k+1}^z$$

$h_x = 1$ $\quad h_z = 0.5$ Chaotic case

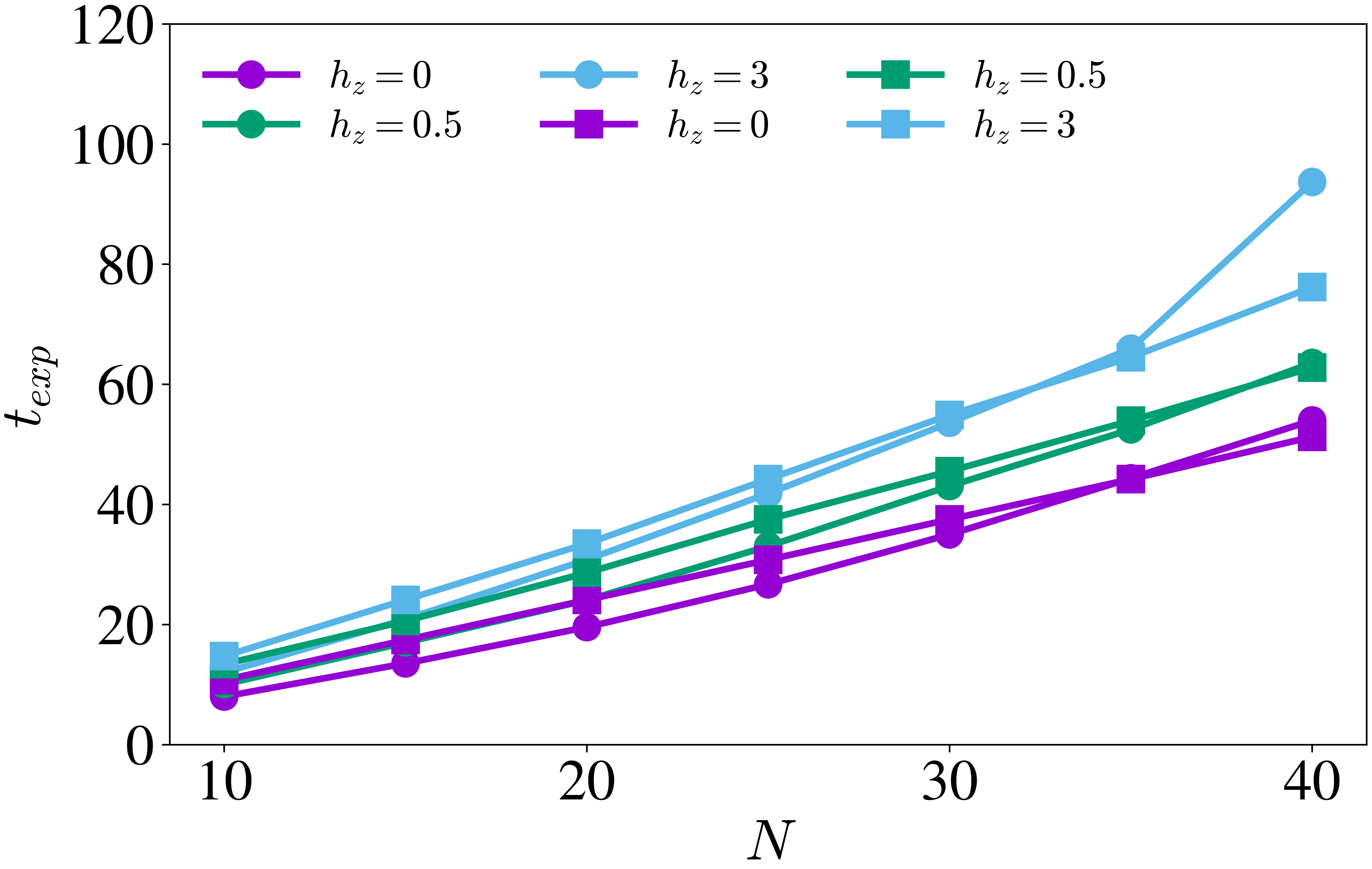
$h_z = 0$

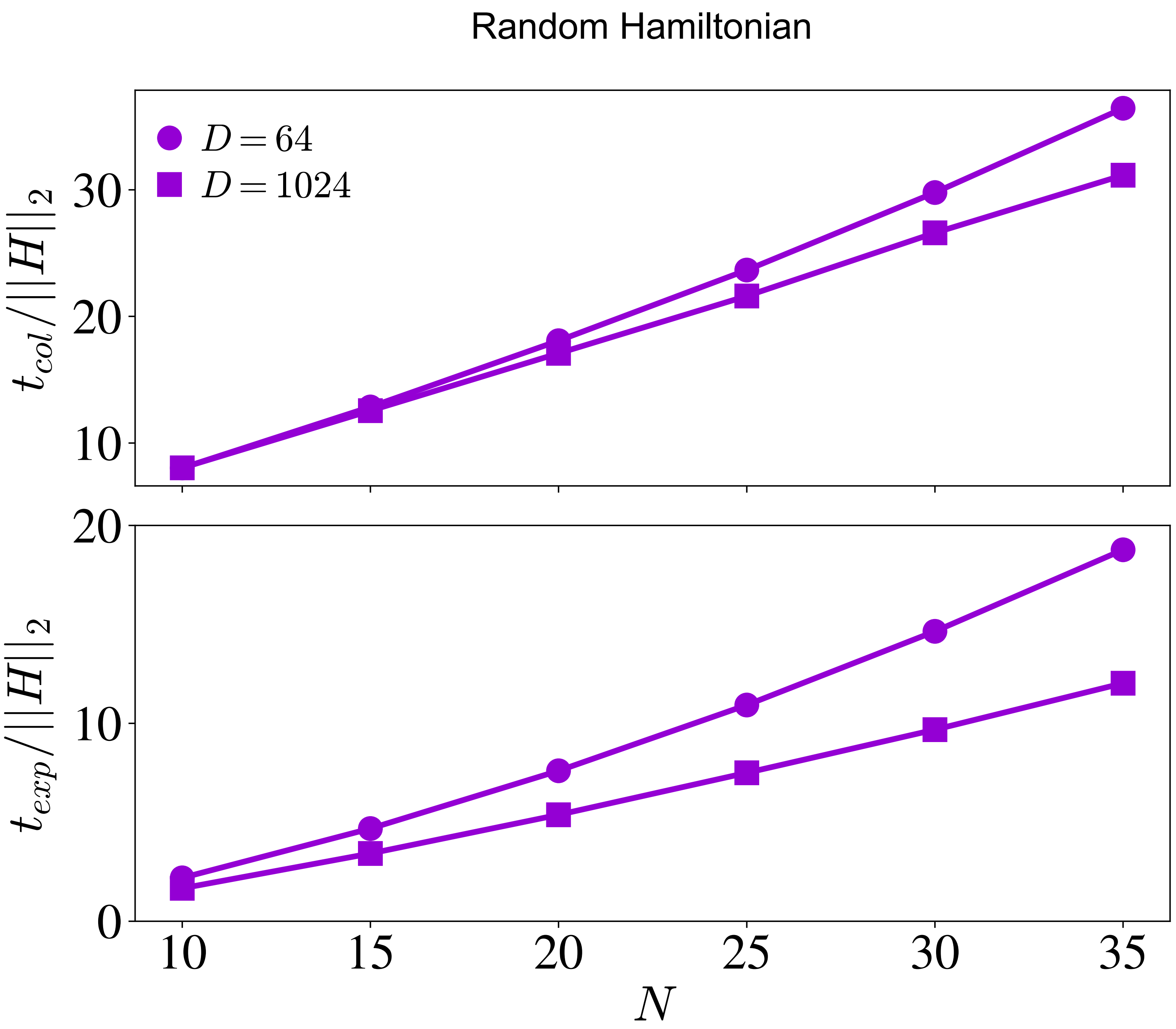
$h_z = 10$

} Integrable case



10^{0}
10^{-4}
10^{-8}
10^{-12}
10^{-16}
$\varepsilon_N(t)$
0
20
40
60
80
$t(time)$
Integrable spin chain


$h_z = 0$
$h_z = 3$
$h_z = 0.5$
$h_z = 0.5$
$h_z = 0$
$h_z = 3$
120
100
80
60
40
20
0
t_{exp}
10
20
30
40
N



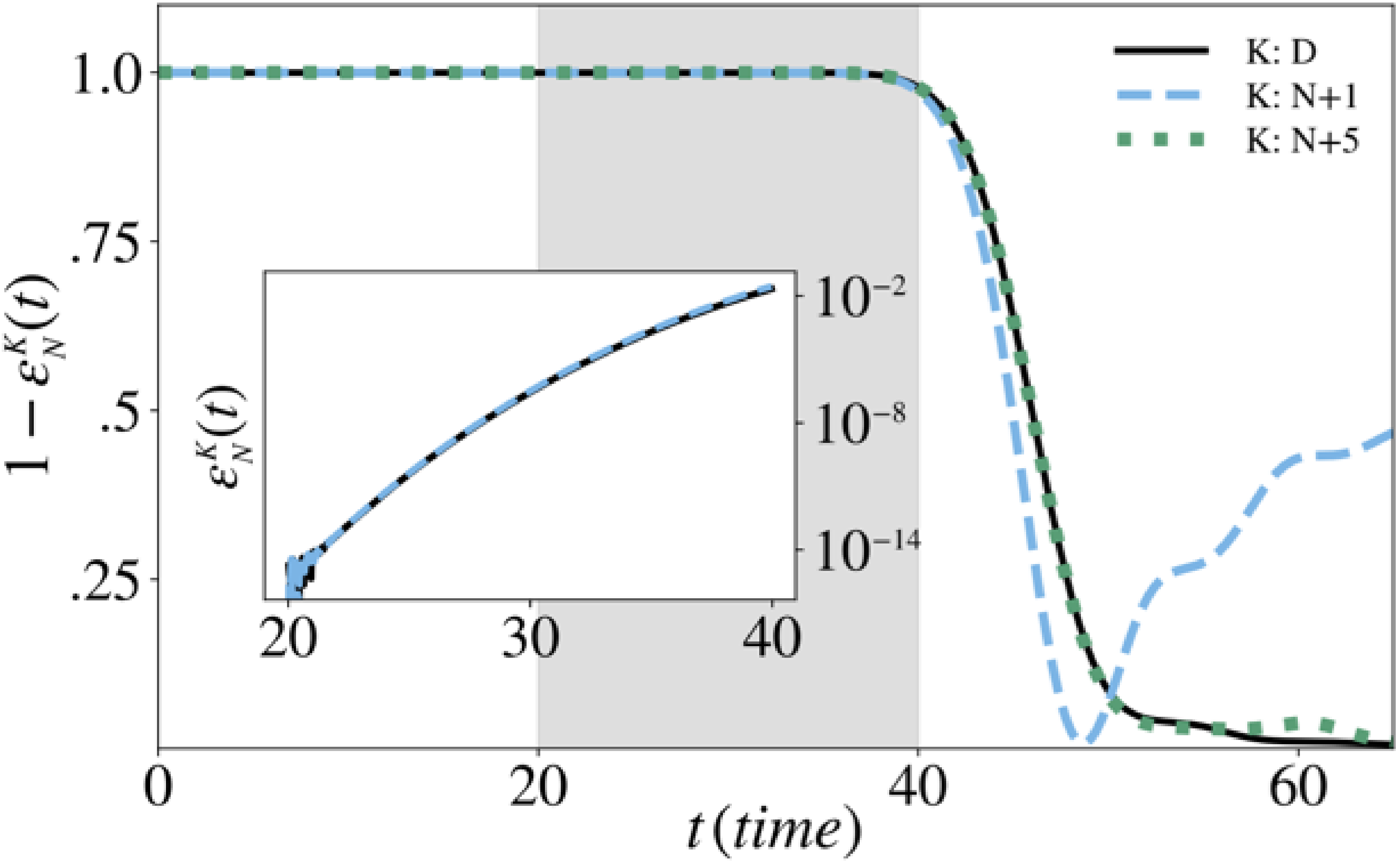
Random Hamiltonian
$D = 64$
$D = 1024$
$t_{col}/||H||_2$
$t_{exp}/||H||_2$
10
20
30
0
10
20
10
15
20
25
30
35
N

From Loschmidt Echoes to Error Bounds

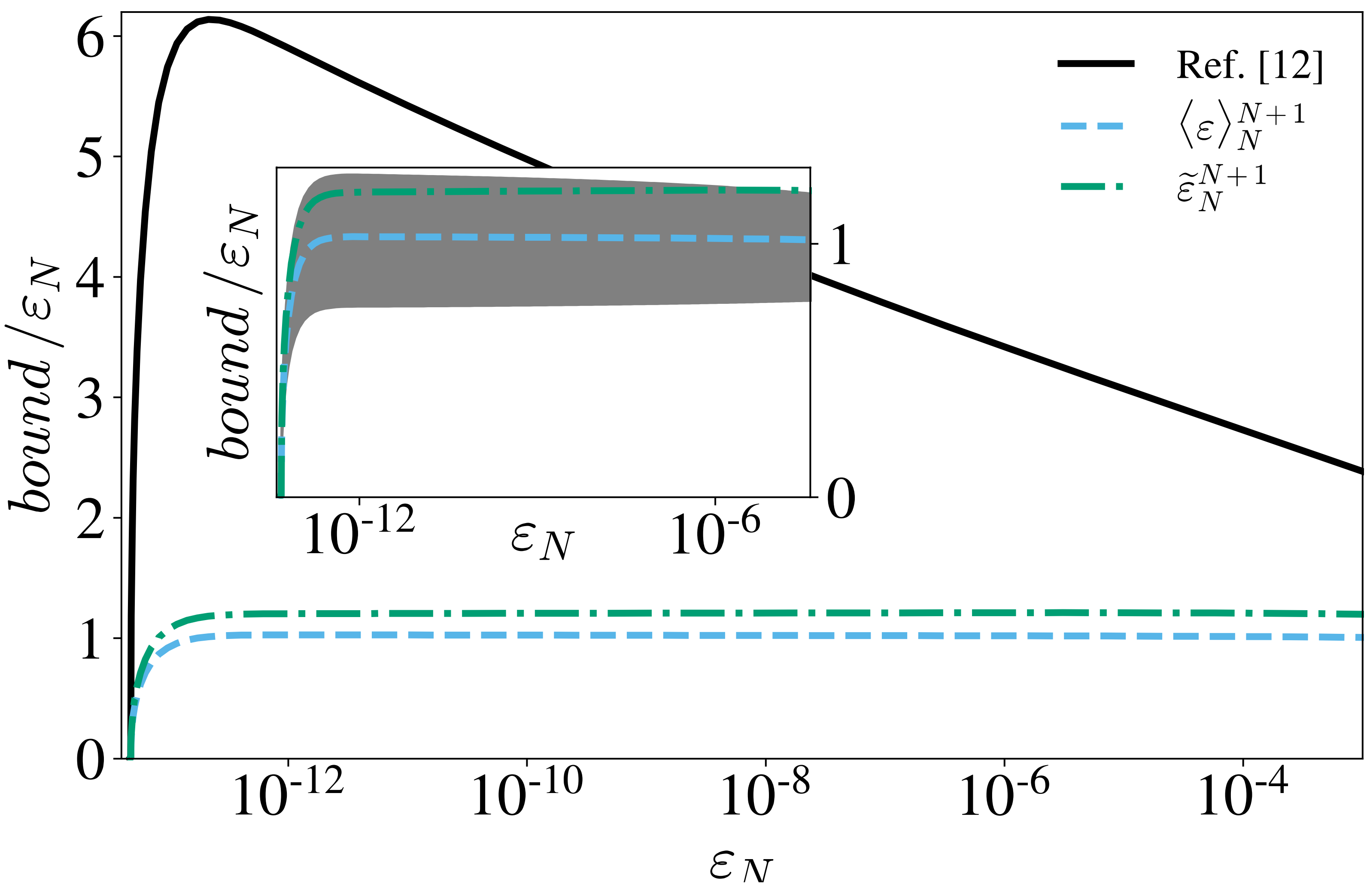
$$|\langle\psi_N(t)|\psi(t)\rangle|^2 \qquad |\langle\psi_N(t)|\psi_K(t)\rangle|^2$$

This is what we want

We ask if this describes the error



K: D
K: N+1
K: N+5
1.0
.75
.5
.25
$1-\varepsilon_N^K(t)$
$\varepsilon_N^K(t)$
10^{-2}
10^{-8}
10^{-14}
20
30
40
0
20
40
60
$t\,(time)$



Ref. [12]
$\langle \varepsilon \rangle_N^{N+1}$
$\tilde{\varepsilon}_N^{N+1}$
$bound\,/\varepsilon_N$
ε_N
0
1
2
3
4
5
6
10^{-12}
10^{-10}
10^{-8}
10^{-6}
10^{-4}

Krylov en Qutip!!!

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Krylov subspace method

Quantum evolution of states

K-complexity

Efficient evolution: we find an error bound using the connection with Loschmidt echo

Evolution of operators

K-complexity

Long-time and quantum chaos

Time dependent quantities or dynamical signatures of Q. Ch.

- Loschmidt echo
- Survival probability
- Purity
- OTOC
- K-complexity

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A Universal Operator Growth Hypothesis

Daniel E. Parker,[1,*] Xiangyu Cao,[1,†] Alexander Avdoshkin,[1,‡] Thomas Scaffidi,[1,2,§] and Ehud Altman[1,¶]

[1]*Department of Physics, University of California, Berkeley, California 94720, USA*
[2]*Department of Physics, University of Toronto, Toronto, Ontario M5S 1A7, Canada*

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We present a hypothesis for the universal properties of operators evolving under Hamiltonian dynamics in many-body systems. The hypothesis states that successive Lanczos coefficients in the continued fraction expansion of the Green's functions grow linearly with rate α in generic systems, with an extra logarithmic correction in 1D. The rate α—an experimental observable—governs the exponential growth of operator complexity in a sense we make precise. This exponential growth prevails beyond semiclassical or large-N limits. Moreover, α upper bounds a large class of operator complexity measures, including the out-of-time-order correlator. As a result, we obtain a sharp bound on Lyapunov exponents $\lambda_L \leq 2\alpha$, which complements and improves the known universal low-temperature bound $\lambda_L \leq 2\pi T$. We illustrate our results in paradigmatic examples such as nonintegrable spin chains, the Sachdev-Ye-Kitaev model, and classical models. Finally, we use the hypothesis in conjunction with the recursion method to develop a technique for computing diffusion constants.

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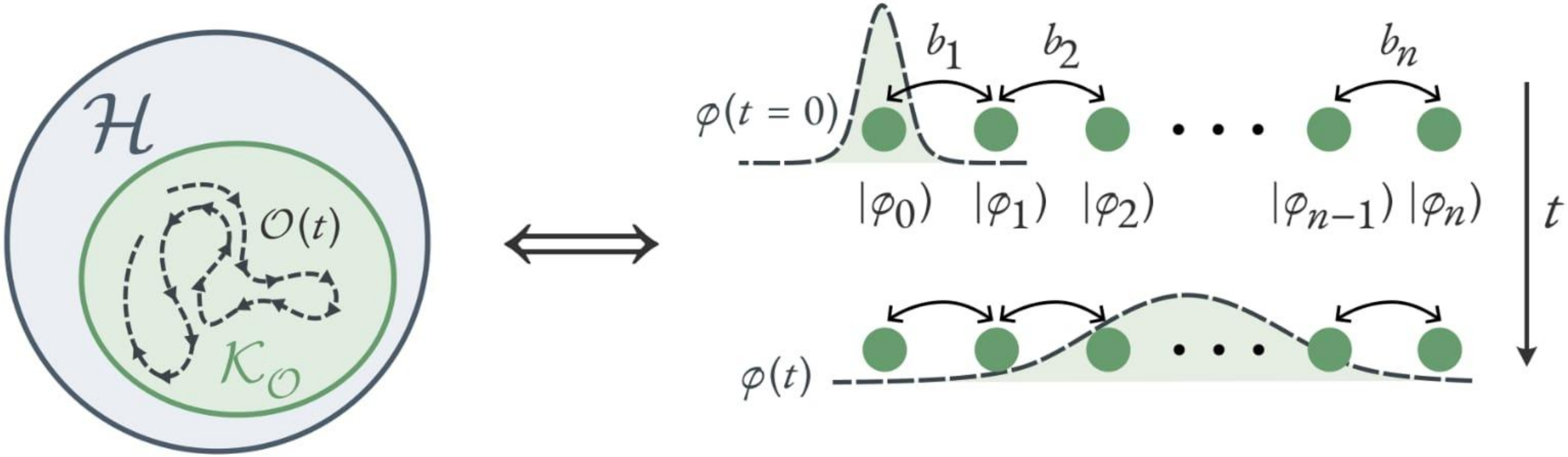
Subject Areas: Condensed Matter Physics, Nonlinear Dynamics, Quantum Physics

Operator dynamics in many-body systems



$\mathcal{H}$
$\mathcal{O}(t)$
$\mathcal{K}_\mathcal{O}$
$\varphi(t=0)$
b_1
b_2
b_n
$|\varphi_0)$
$|\varphi_1)$
$|\varphi_2)$
$|\varphi_{n-1})$
$|\varphi_n)$
t
$\varphi(t)$

Krylov subspace, Lanczos algorithm and K-complexity

H

Hamiltonian

$\mathcal{O}$

hermitian operator

$\mathcal{L} = [H, \cdot]$

Liouvillian superoperator

$\mathcal{O}(t)$

$$\mathcal{O}(t) = e^{iHt}\mathcal{O}e^{-iHt} = \sum_{n=0}^{\infty} \frac{(it)^n}{n!} \mathcal{L}^n \mathcal{O}$$

the Krylov subspace is defined as the minimum subspace of L that contains O(t) at all time

$$\mathcal{K} = \mathrm{span}\{|\mathcal{O}),\ \mathcal{L}|\mathcal{O}),\ \mathcal{L}^2|\mathcal{O}), \cdots\}$$

$$\mathcal{L}\,|\mathcal{O}) = b_n|\mathcal{O}_{n-1}) + b_{n+1}\,|\mathcal{O}_{n+1})$$

$$(\mathcal{O}_n|\mathcal{L}|\mathcal{O}_m) = \begin{pmatrix} 0 & b_1 & 0 & 0 & \cdots \\ b_1 & 0 & b_2 & 0 & \cdots \\ 0 & b_2 & 0 & b_3 & \cdots \\ 0 & 0 & b_3 & 0 & \ddots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix}$$

$$|\mathcal{O}(t)) = \sum_{n=0}^{K-1} i^n\,\phi_n(t)\,|\mathcal{O}_n)$$

$$\partial_t\phi_n(t) = b_n\phi_{n-1} - b_{n+1}\,\phi_{n+1}$$

K-complexity

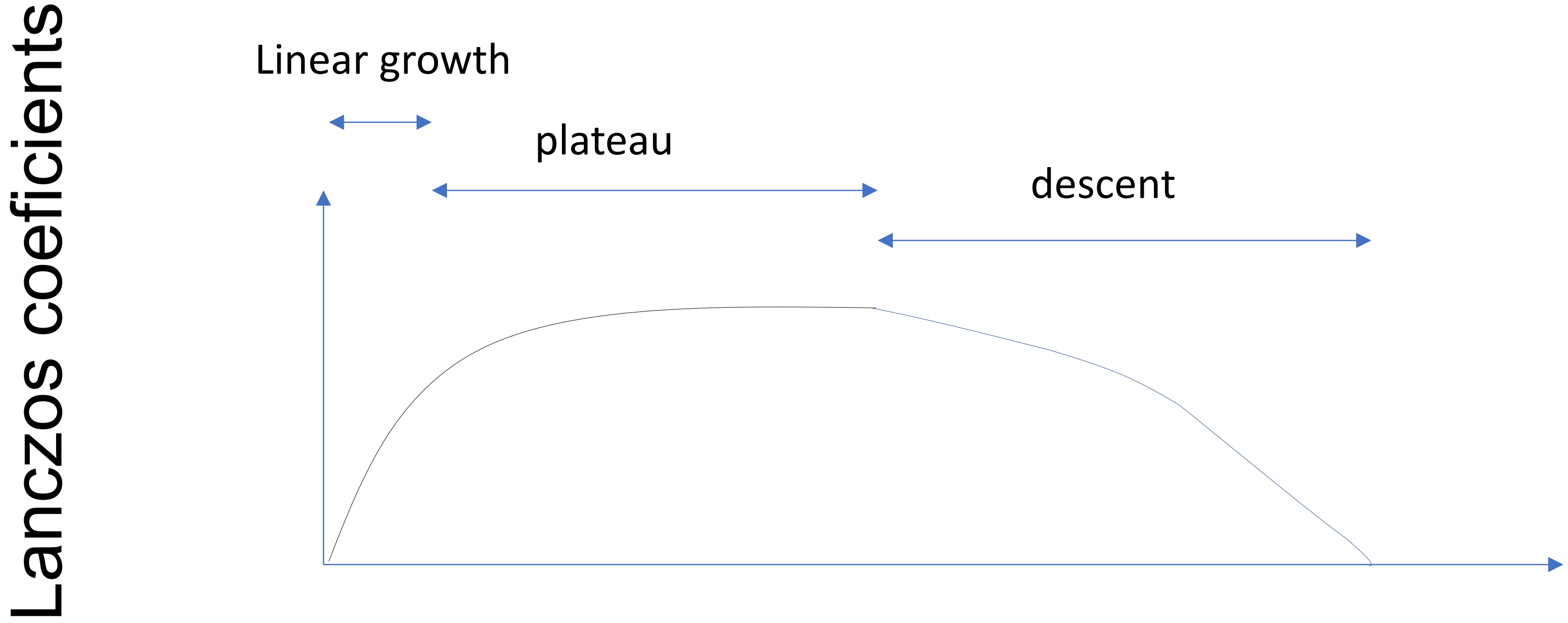
the time-dependent average position over the Krylov chain

$$\mathcal{K}_C(t) = \sum_{n=0}^{K-1} n \left|\phi_n(t)\right|^2$$

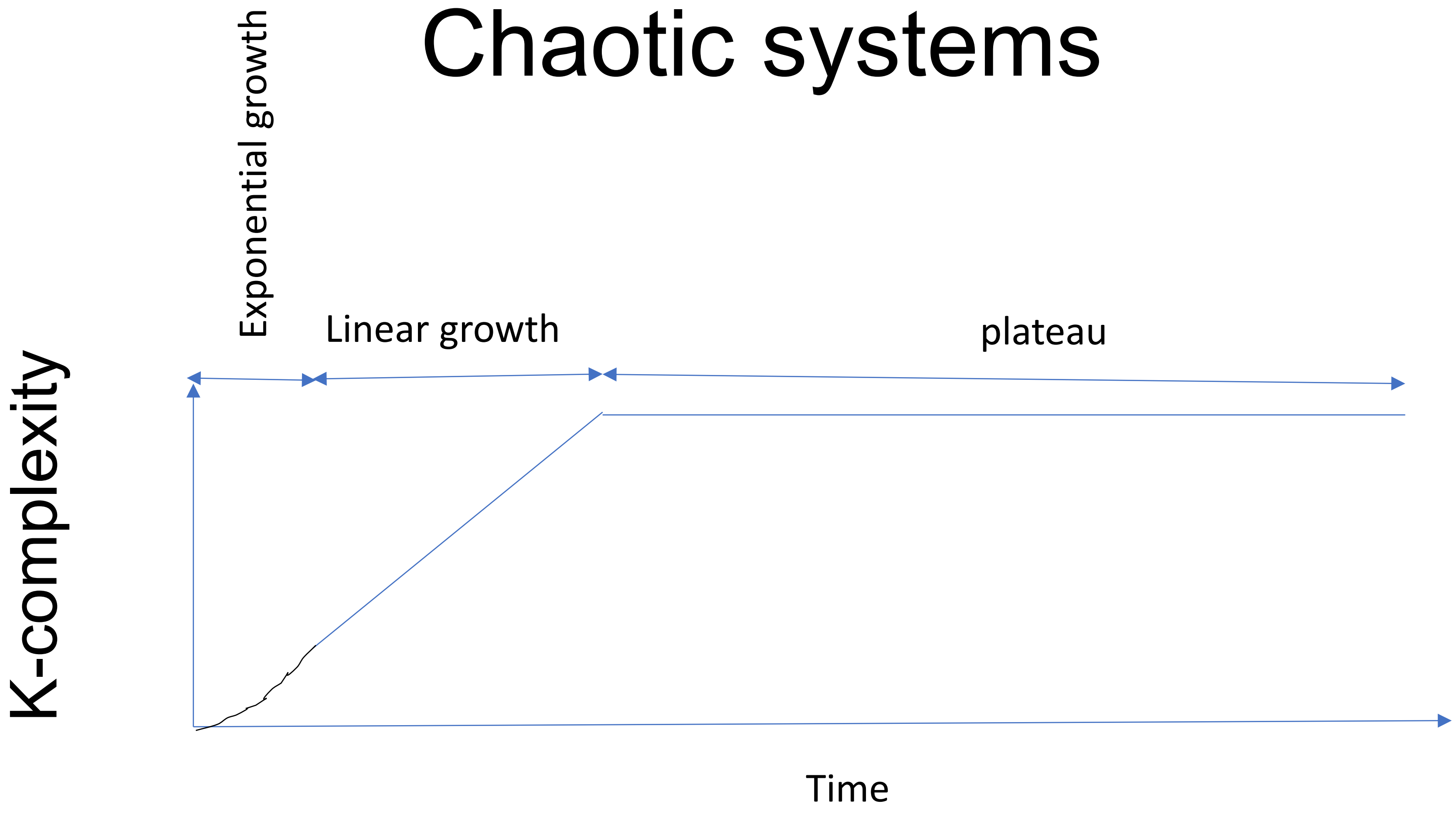
$$\overline{\mathcal{K}_C} = \sum_{n=0}^{K-1} n \overline{\left|\phi_n(t > \tau)\right|^2}$$

τ the time at which complexity saturates

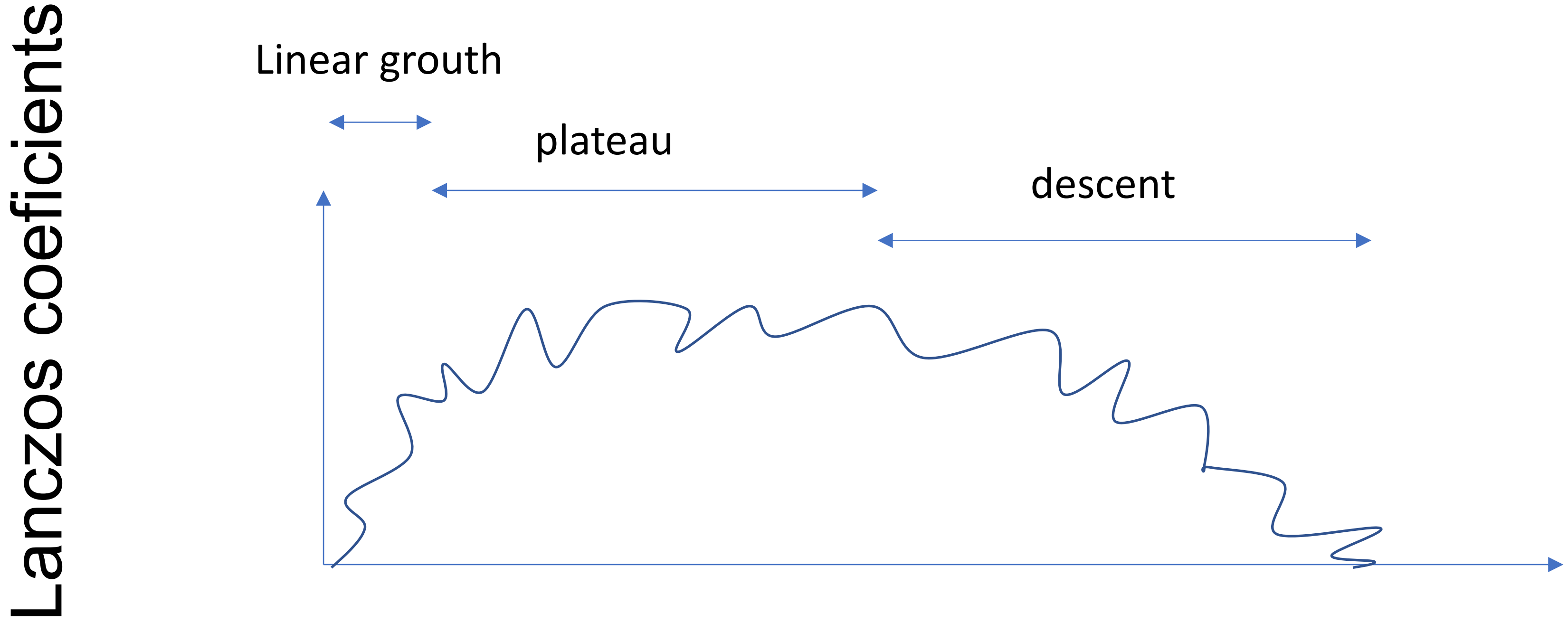
Chaotic systems



Chaotic systems



Integrable systems



More fluctuation in b_n ➡ evolution in tight-binding chain with more disorder

➡ Anderson localization ➡ Lower K-complexity

Ising spin chain with transverse magnetic field

$$\hat{H}_E = \sum_{k=1}^{L} \left(h_x \hat{\sigma}_k^x + h_z \hat{\sigma}_k^z \right) - J \sum_{k=1}^{L-1} \hat{\sigma}_k^z \hat{\sigma}_{k+1}^z$$

Medida de caos espectral

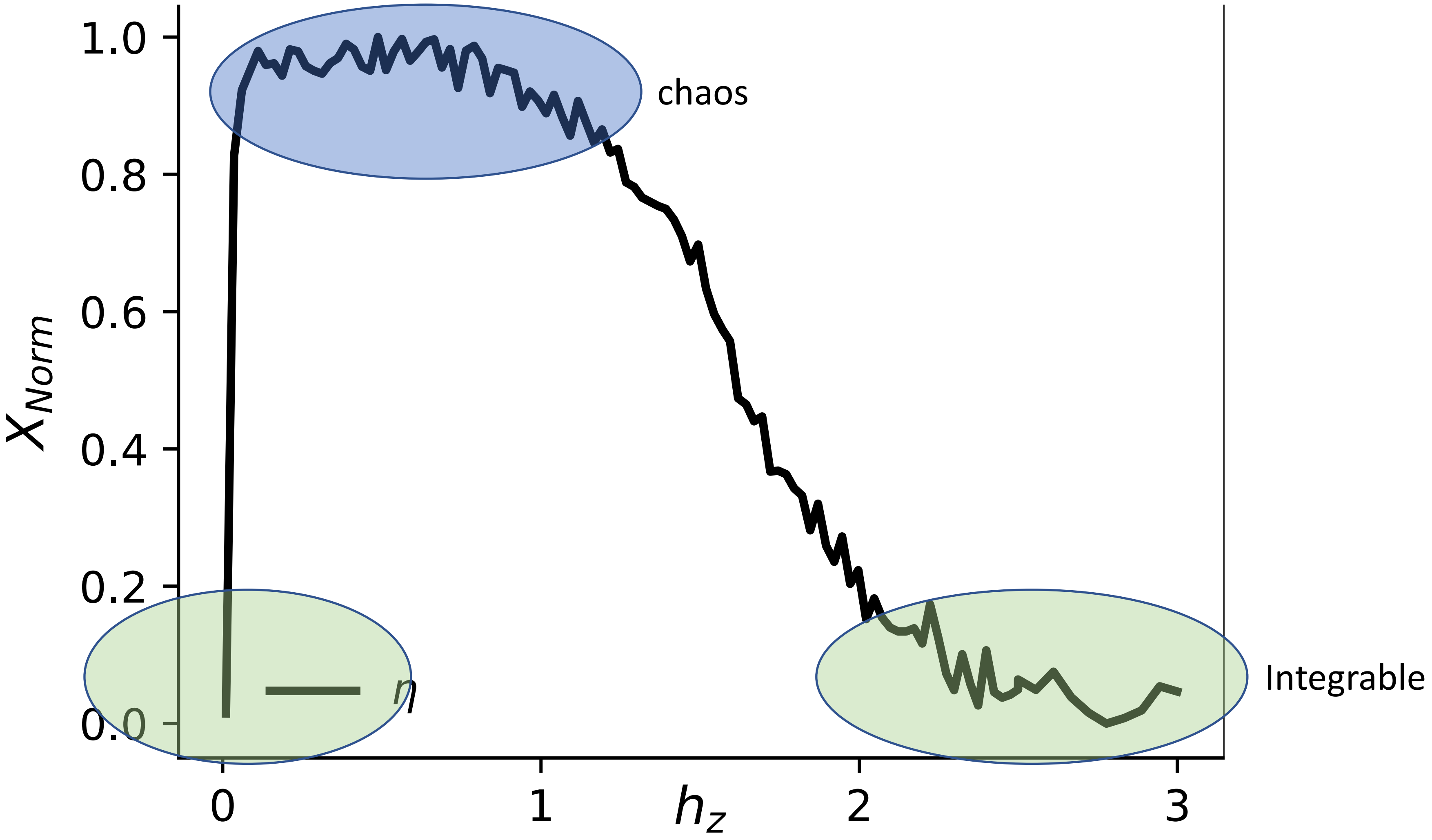
$$s_i = e_i - e_{i-1}$$

$$\langle \tilde{r} \rangle = \frac{1}{D} \sum_{n=1}^{D} \tilde{r}_n; \qquad \tilde{r}_n = \frac{\min(s_n, s_{n-1})}{\max(s_n, s_{n-1})}$$

$$\langle \tilde{r} \rangle_P \approx 0.38629$$

$$\langle \tilde{r} \rangle_{WD} \approx 0.53590$$

$$\eta = \frac{\langle \tilde{r} \rangle - \langle \tilde{r} \rangle_P}{\langle \tilde{r} \rangle_{WD} - \langle \tilde{r} \rangle_P}$$



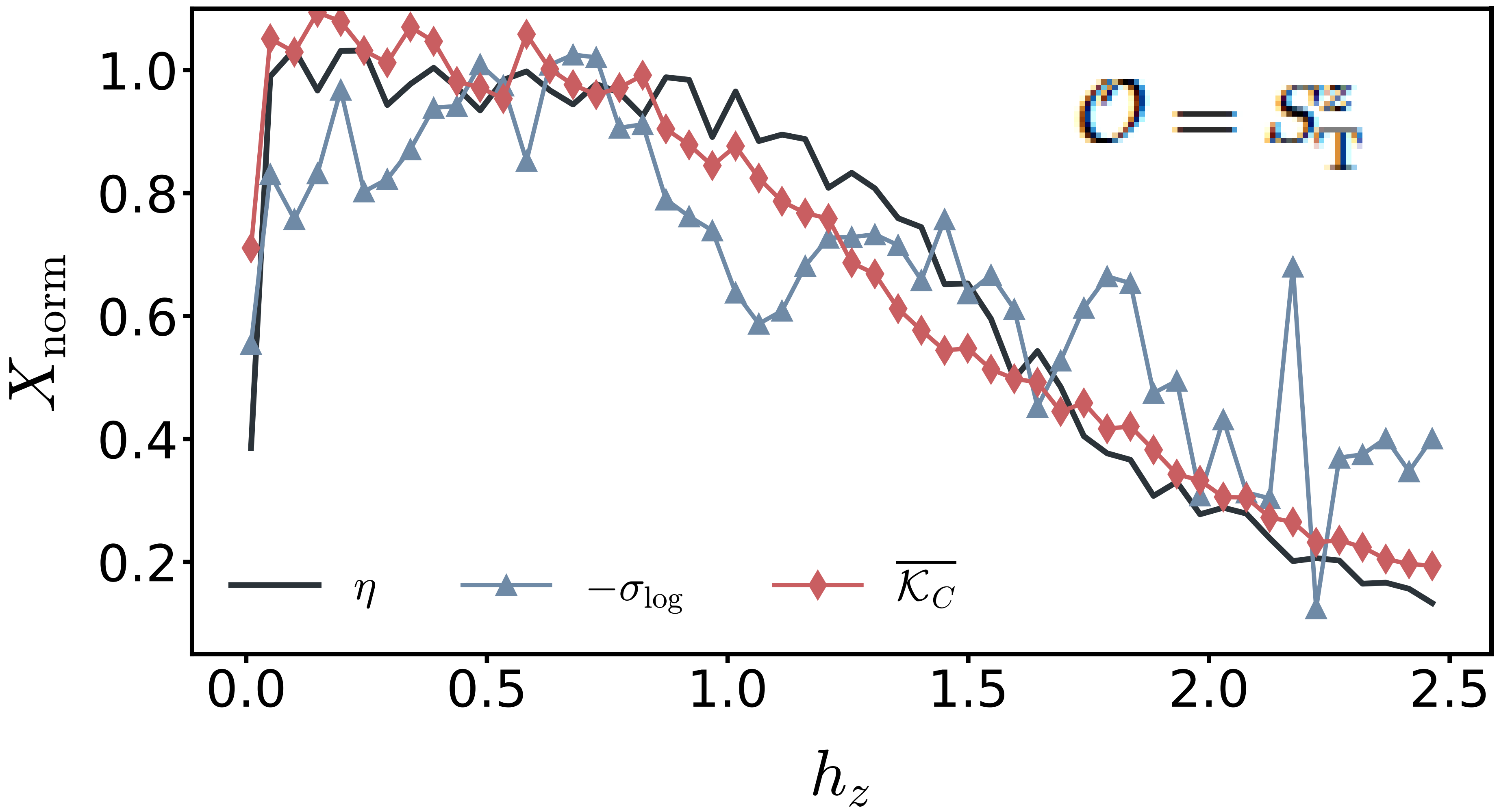
1.0
0.8
0.6
0.4
0.2
0.0
X_{Norm}
chaos
Integrable
η
0
1
h_z
2
3

From integrability to chaos through Lanczos Coefficients

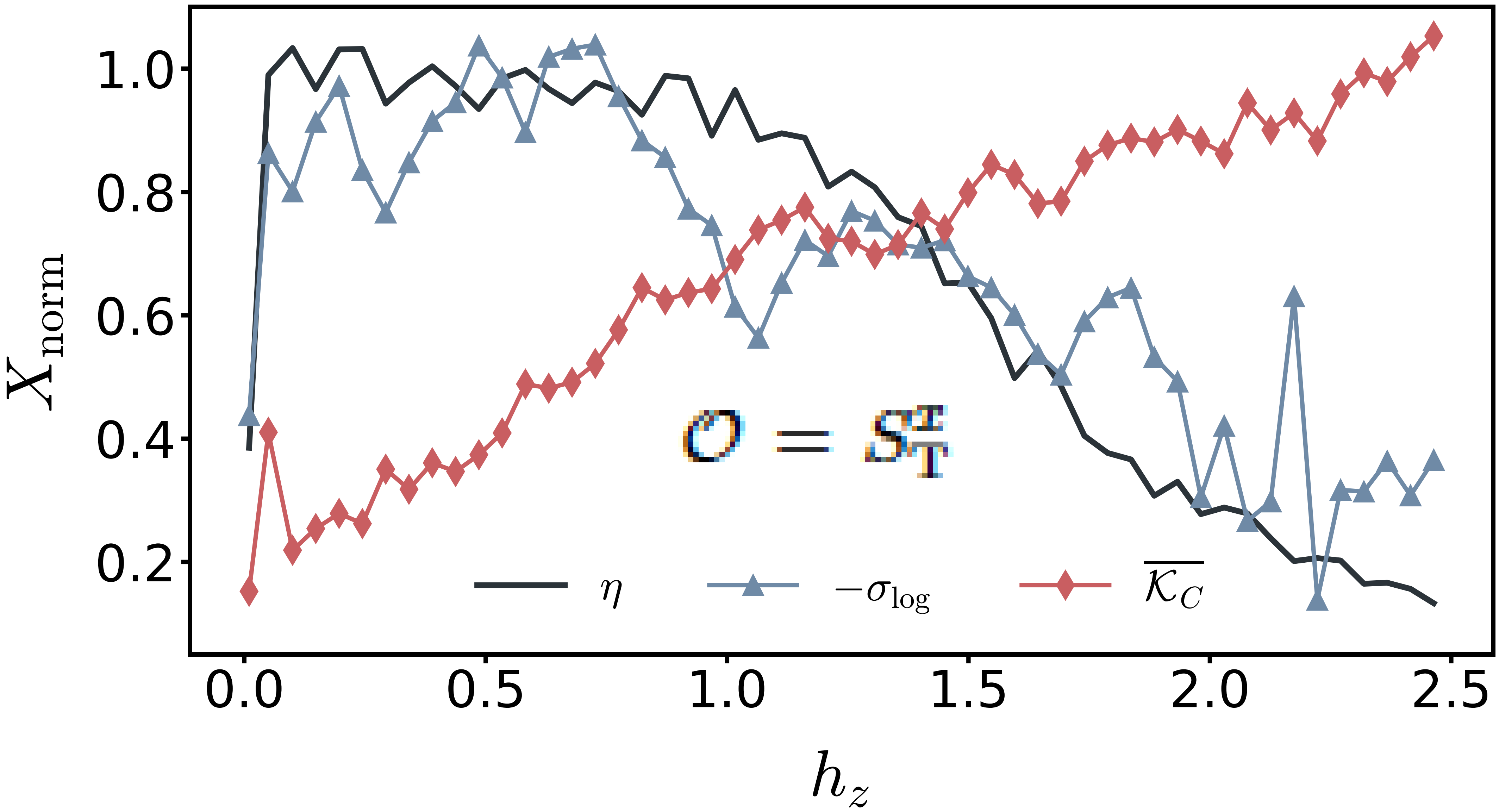
Operators $$S_{\mathrm{T}}^{\alpha} = \sum_{k=1}^{L} \frac{1}{2} \sigma_k^{\alpha} \qquad \alpha = \{x, y, z\}$$

Measure of the dispersion of the Lanczos coefficients

$$\sigma_{\log} = \mathrm{STD}\{\log(b_n) - \log(b_{n+1})\} = \mathrm{STD}\{\log(b_n/b_{n+1})\}$$



$\mathcal{O} = S^z_{\mathrm{T}}$
X_{norm}
h_z
η
$-\sigma_{\log}$
$\overline{\mathcal{K}_C}$
1.0
0.8
0.6
0.4
0.2
0.0
0.5
1.0
1.5
2.0
2.5



X_{norm}
1.0
0.8
0.6
0.4
0.2
0.0
0.5
1.0
1.5
2.0
2.5
h_z
$O = S^{z}_{T}$
η
$-\sigma_{\log}$
$\overline{\mathcal{K}_C}$

Complejidad de Krylov para estados

$$|\psi(t)\rangle = e^{-itH}\,|\psi_0\rangle = \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} H^n\,|\psi_0\rangle$$

$$K = \mathrm{span}\{H^n\,|\psi_0\rangle\}_{n=0}^{K-1}$$

$$|A_{n+1}\rangle = (H - a_n)\,|K_n\rangle - b_n\,|K_{n-1}\rangle\,, \quad |K_n\rangle = b_n^{-1}\,|A_n\rangle$$

$$a_n = \langle K_n|\,H\,|K_n\rangle\,, \quad b_n = \sqrt{\langle A_n|A_n\rangle}$$

$$H\,|K_n\rangle = a_n\,|K_n\rangle + b_{n+1}\,|K_{n+1}\rangle + b_n\,|K_{n-1}\rangle$$

$$|\psi(t)\rangle = \sum_{n=0}^{K-1} \psi_n(t)\,|K_n\rangle$$

$$i\partial_t \psi_n(t) = a_n \psi_n(t) + b_n \psi_{n-1}(t) + b_{n+1} \psi_{n+1}(t)$$

$$\boxed{C_K(t) = \sum_{n=0}^{K-1} n|\psi_n(t)|^2}$$

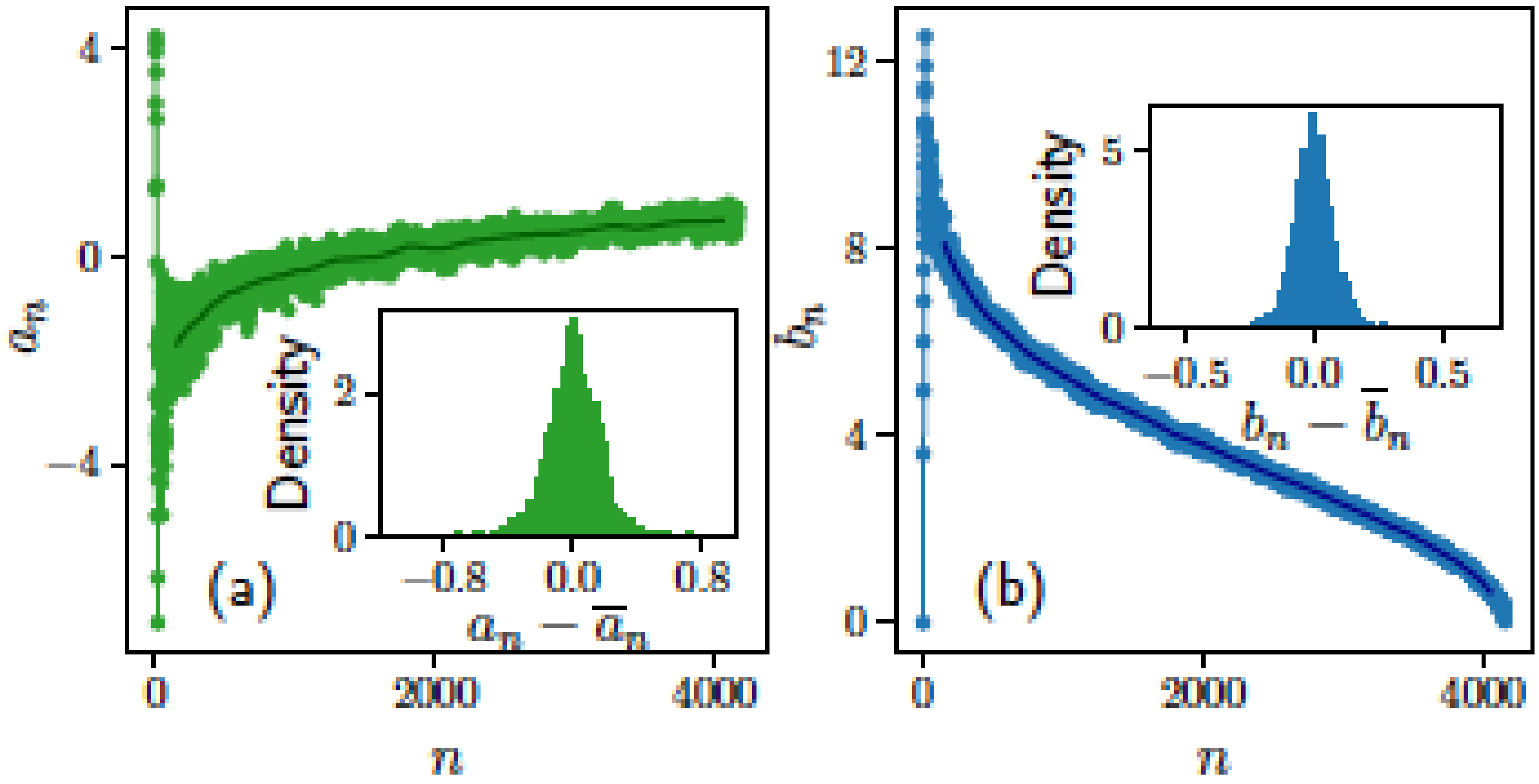
$$\overline{C_{\mathcal{K}}} \equiv \lim_{T\to\infty} \frac{1}{T} \int_0^T dt\, C_{\mathcal{K}}(t) = \sum_{n=0}^{D-1} n Q_{0n}$$

$$Q_{0n} \equiv \sum_{i=1}^{D} |\langle e_i|\psi_0\rangle|^2 |\langle K_n|e_i\rangle|^2$$

$$e_i \varepsilon_n^i = a_n \varepsilon_n^i + b_n \varepsilon_{n-1}^i + b_{n+1} \varepsilon_{n+1}^i$$

$$\overline{C_{\mathcal{K}}} = \frac{1}{D} \sum_{n=0}^{D-1} n = \frac{D-1}{2}$$

$$\sigma^2(s_n) \equiv \frac{1}{N} \sum_{n=n_0}^{N} (s_n - \overline{s}_n)^2, \text{ with } \overline{s}_n = \frac{1}{2w} \sum_{m=n-w}^{n+w} s_m.$$



Cadena de spines

$$H = \sum_{i=1}^{N} \left(\sigma_x^{(i)} + h_z \sigma_z^{(i)} \right) - \sum_{i=1}^{N-1} \sigma_z^{(i)} \sigma_z^{(i+1)}$$

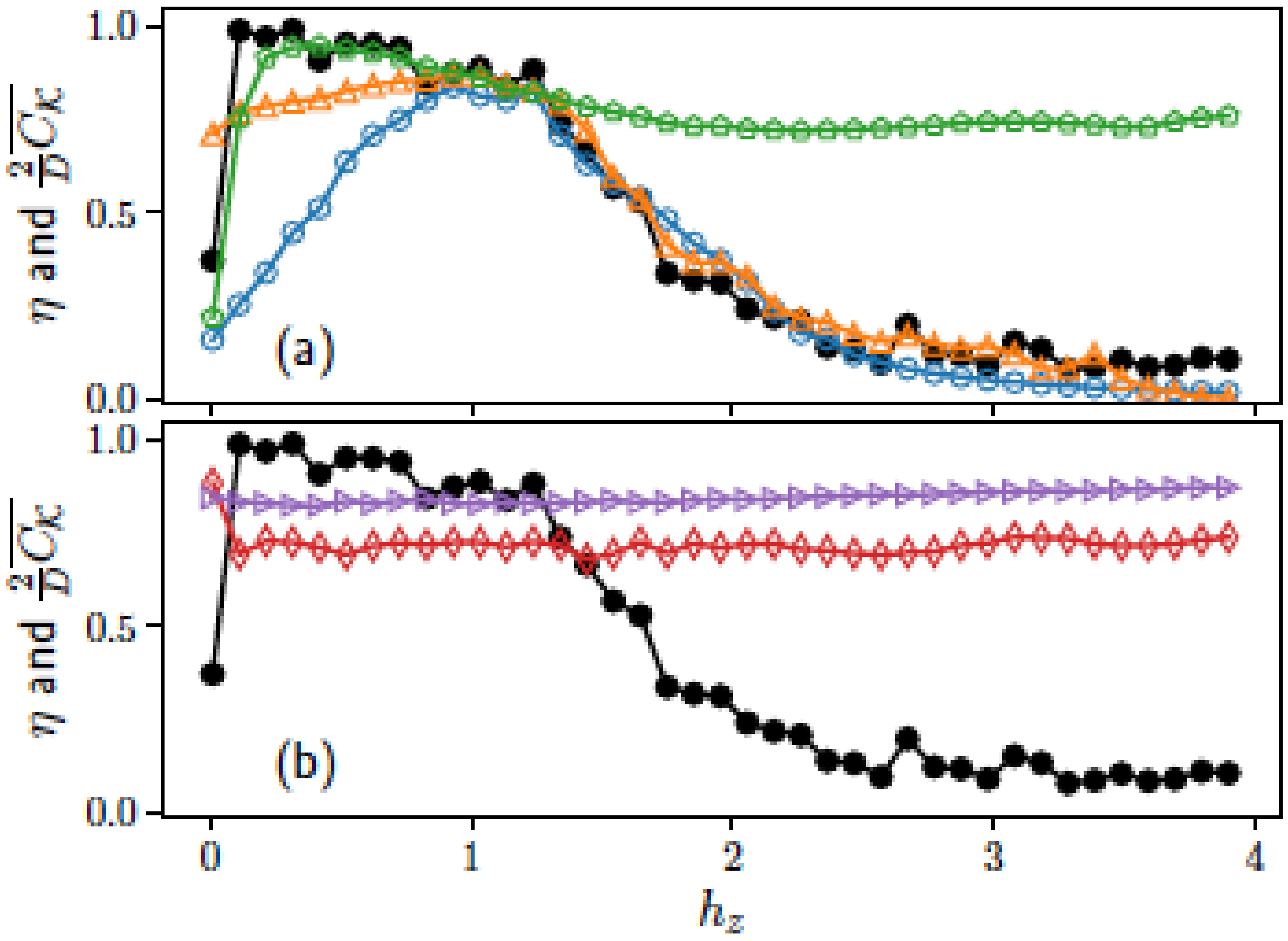
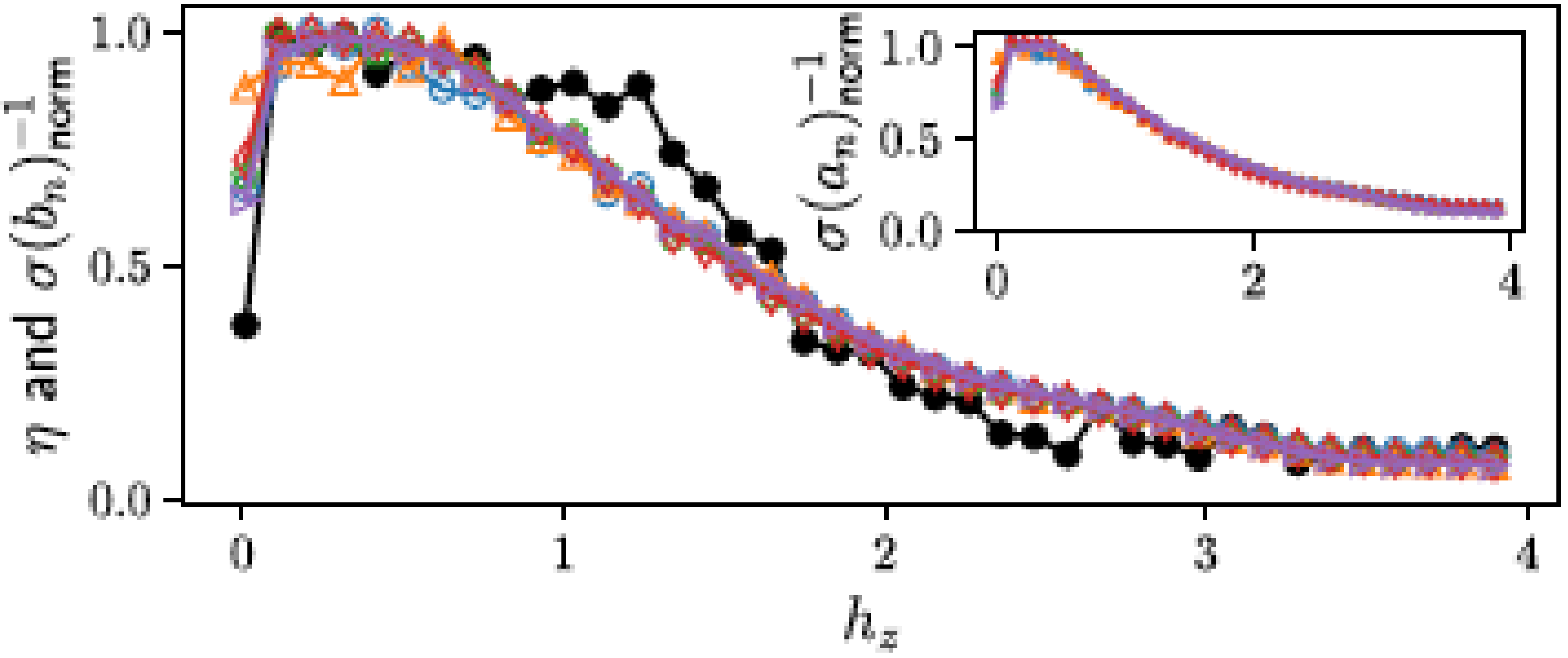


FIG. 3. Chaotic measure η (black filled circles) and saturation of the $\mathcal{K}$-complexity as a function of the chaos parameter h_z through the chaos-to-integrability transition in the Ising spin chain for a variety of initial states. The complexity curves correspond to (a) an initial state in the all spins 'up' configuration (blue circles), an average over initial states from the eigenbasis of the integrable Hamiltonian with $h_z = 4$ (orange triangles), and an average over initial states from the eigenbasis of the integrable Hamiltonian with $h_z = 0$ (green pentagons), (b) average over random initial states (red diamonds) and an initial state uniformly distributed over the eigenbasis of the integrable Hamiltonian with $h_z = 0$ (purple triangles).



1.0
0.5
0.0
0
1
2
3
4
h_z
η and $\sigma(b_n)^{-1}_{\text{norm}}$
$\sigma(a_n)^{-1}_{\text{norm}}$
1.0
0.5
0.0
0
2
4

Modelo de matrices aleatorias

$$H_{\mathrm{RMT}} = \frac{H_0 + kV}{\sqrt{1+k^2}}$$

where H_0 is a diagonal matrix with elements drawn from a normal distribution with zero mean and unity variance, and V a real banded random matrix of bandwidth b [27]. Hence, this model exhibits a transition from Poissonian level statistics at $k=0$ to GOE when k reaches a sufficiently large value.

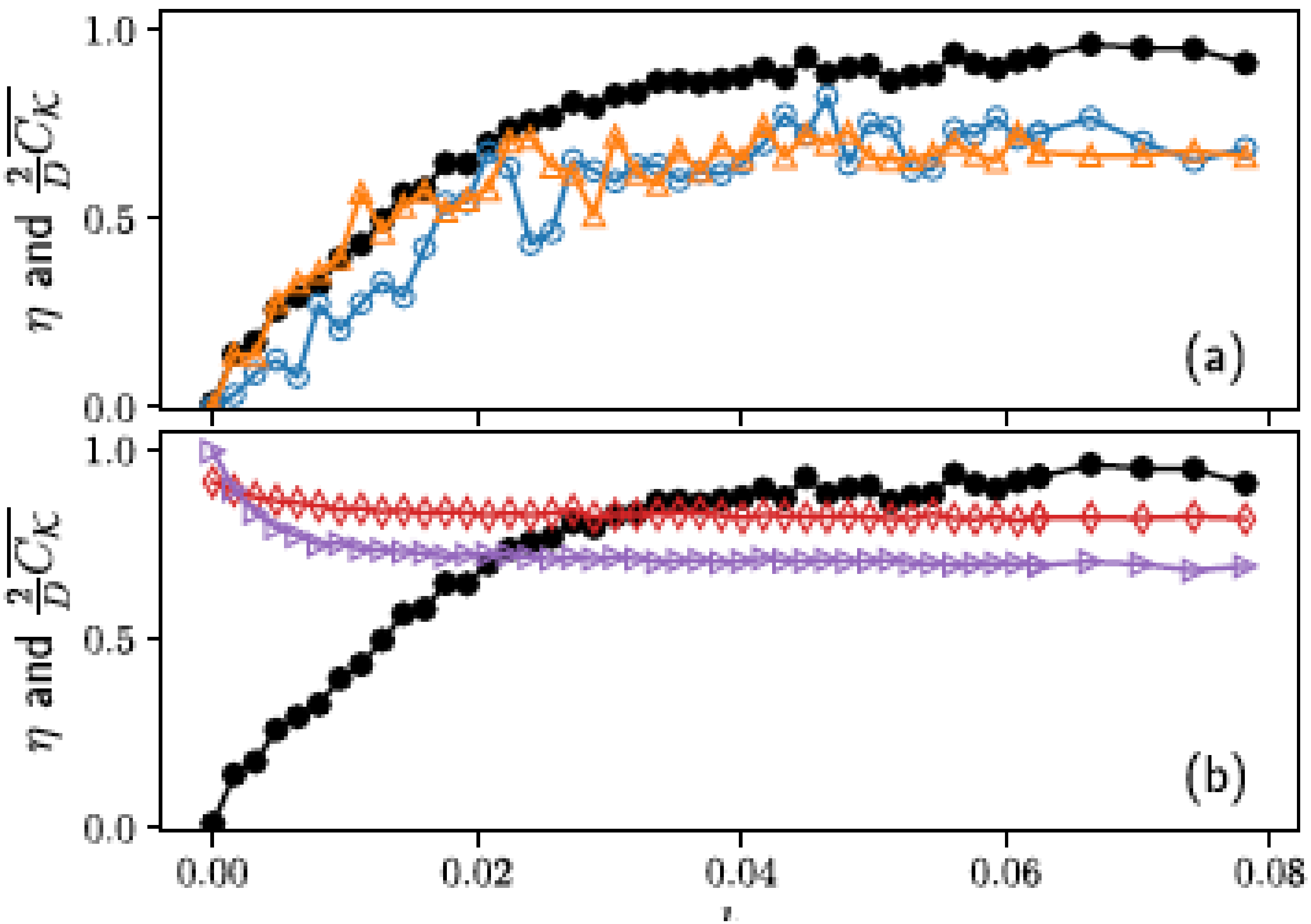
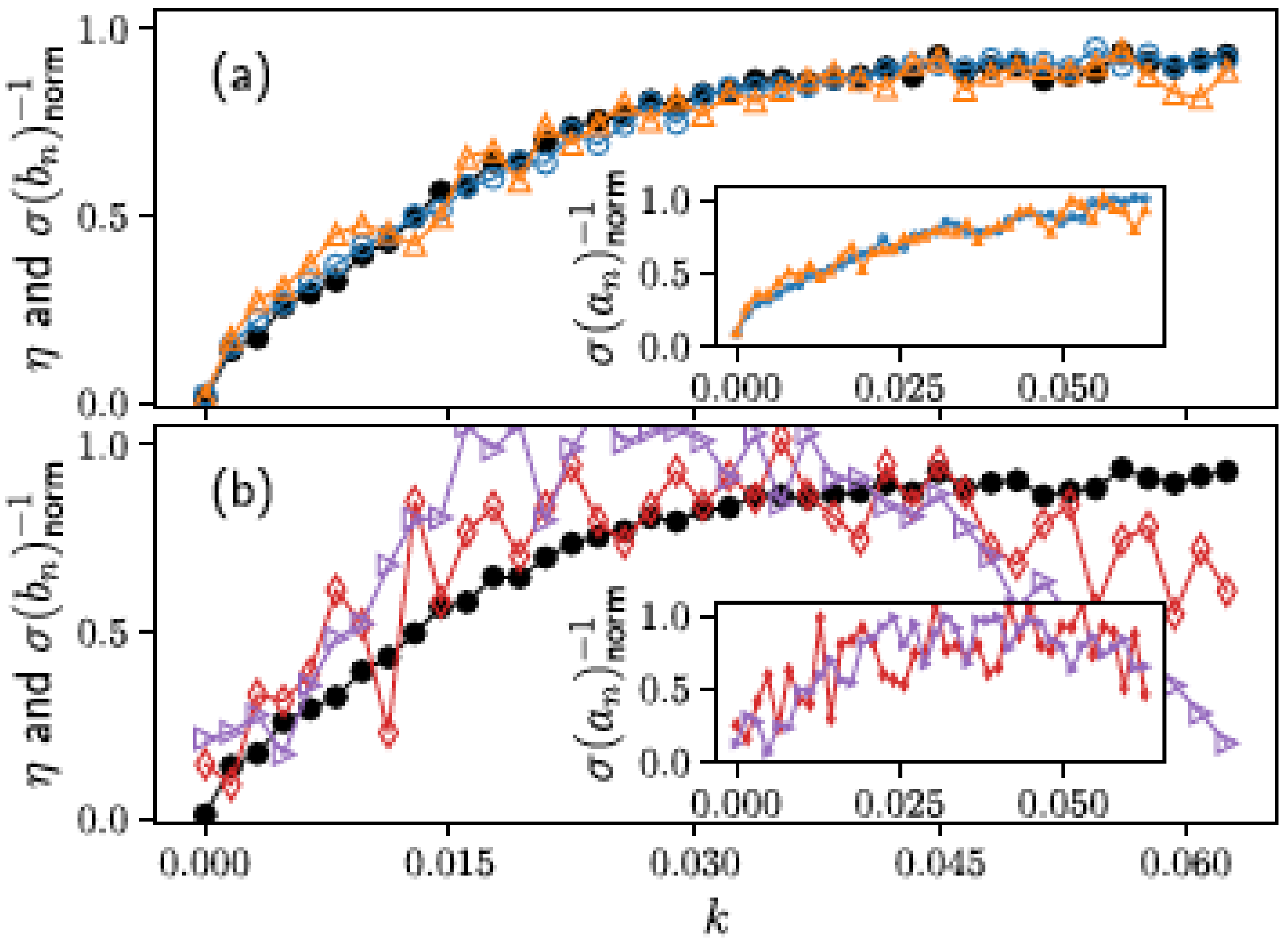


FIG. 5. Chaotic measure η (black filled circles) and saturation of the $\mathcal{K}$-complexity as a function of the chaos parameter k through the Poisson-to-GOE ensemble transition for the banded random matrix model for a variety of initial states. The curves for the Krylov complexity correspond to (a) an initial state that is an eigenstate of $H_{\rm RMT}$ with $k = 0$ in the border of its spectrum (blue circles), an average over initial states from the eigenbasis of $H_{\rm RMT}$ with $k = 0$ (orange triangles), (b) an average over random initial states (red diamonds), and an initial state uniformly distributed over the eigenbasis of $H_{\rm RMT}$ with $k = 0$ (purple triangles).



(a)
(b)
η and σ(b_n)^{-1}_norm
σ(a_n)^{-1}_norm
k
0.0
0.5
1.0
0.000
0.015
0.030
0.045
0.060
0.025
0.050

Complejidad de Krylov para evoluciones unitarias

Arnoldi iteration method

$$|\psi_0\rangle \qquad U \qquad |\psi_t\rangle = U^t|\psi_0\rangle \qquad t \in \mathbb{N}_0$$

$$\{|\psi_0\rangle, |\psi_1\rangle, \ldots\}$$

$$\{|K_0\rangle, |K_1\rangle, \ldots\} \qquad |K_0\rangle = |\psi_0\rangle \qquad \langle K_n|K_m\rangle = \delta_{nm}$$

$$b_n|K_n\rangle = U|K_{n-1}\rangle - \sum_{l=0}^{n-1}\langle K_l|U|K_{n-1}\rangle|K_l\rangle$$

Written in the Krylov basis, the unitary U attains an upper Hessenberg form, since $\langle K_m|U|K_n\rangle = 0$ for any $m > n+1$.

$$b_n = \langle K_n | U | K_{n-1} \rangle, \quad a_n = \langle K_n | U | K_n \rangle$$
$$c_n = \langle K_0 | U | K_n \rangle.$$

$$|K_n\rangle = \sum_{t=0}^{n} \alpha_{n,t} |\psi_t\rangle$$

$$|\psi_t\rangle = \sum_{n=0}^{t} \beta_{t,n} |K_n\rangle$$

$$\langle \psi_t | K_n \rangle = 0 \, \forall t < n \quad \Rightarrow \quad \langle K_m | U | K_n \rangle = \alpha^*_{m\,0} c_n \, \forall m \leqslant n$$

$$\Rightarrow \quad a_m = \alpha^*_{m\,0} c_m$$

$$\Rightarrow \quad \langle K_m | U | K_n \rangle = \frac{a_m}{c_m} c_n \quad \forall m \leqslant n$$

$$p_n(U) = \sum_{t=0}^{n} \alpha_{n,t} U^t$$

$$\frac{1}{2\pi} \int d\varphi \, w(\varphi) p_m(z)^* p_n(z) = \delta_{mn}$$

$$\frac{1}{2\pi} \int d\varphi \, w(\varphi) f(z) = \langle \psi_0 | f(U) | \psi_0 \rangle$$

$$a_n = \frac{1}{2\pi} \int d\varphi \, w(\varphi) e^{i\varphi} |p_n(z)|^2,$$

$$b_n = \frac{1}{2\pi} \int d\varphi \, w(\varphi) e^{i\varphi} p_n(z)^* p_{n-1}(z),$$

$$c_n = \frac{1}{2\pi} \int d\varphi \, w(\varphi) e^{i\varphi} p_n(z).$$

A measure of ergodicity

"maximally ergodic Krylov dynamics"

(se mostro en circuitos)

$$\mathcal{U}O_n = O_{n+1}$$

↓ ↓

Operadores de la base de Krylov

Krylov space is explored most efficiently

A measure of ergodicity

The maximally ergodic regime identified in Ref. [11] arises from the asymptotic behavior for the polynomials (6) which, under some regularity conditions upon the weight function w, satisfy the asymptotic behavior [23]

$$p_n(z) \approx \frac{z^n}{\sqrt{w(\varphi)}} \quad \text{for } n \gg 1. \tag{10}$$

As a consequence, for large n the matrix elements of U in the Krylov basis fulfill the following three properties [11]:

As a consequence, for large n the matrix elements of U in the Krylov basis fulfill the following three properties [11]:

(i) The sequences (9) in this limit are

$$\begin{aligned} a_n &= \frac{1}{2\pi}\int d\varphi\, e^{i\varphi} = 0, \quad b_n = \frac{1}{2\pi}\int d\varphi \, = 1, \\ c_n &= \frac{1}{2\pi}\int d\varphi\, \sqrt{w(\varphi)} e^{i\varphi(n+1)} = f^*_{n+1} \to 0, \end{aligned} \tag{11}$$

where f_n is the nth Fourier coefficient of $\sqrt{w(\varphi)}$. Thus, U becomes purely lower diagonal in the Krylov basis, implying $U|K_n\rangle = |K_{n+1}\rangle$.

(ii) The autocorrelators for the Krylov states $C^{(n)}_t = \langle K_n|U^t|K_n\rangle$, which can be written as

$$C^{(n)}_t = \frac{1}{2\pi}\int d\varphi\, w(\varphi) e^{it\varphi}|p_n(z)|^2, \tag{12}$$

attain the form

$$C^{(n)}_t = \frac{1}{2\pi}\int d\varphi\, e^{it\varphi} = \delta_{t0} \tag{13}$$

such that their autocorrelations decay in a single time step.

(iii) The discrete-time Fourier transforms of these autocorrelations $C^{(n)}_\omega$ become constant, which follows straightforwardly from (13).

A measure of ergodicity

$$\mathrm{Erg}(U)^{-1} = \frac{1}{\sqrt{2\mathrm{Tr}(\mathbb{I})}} \|U_{\mathrm{erg}} - U_{\mathcal{K}}\|_{2,2}.$$

$U^{\mathrm{erg}}_{n,m} = \delta_{n,m+1}$, and $\|\cdot\|_{2,2}$ is the $L_{2,2}$ norm

MEASURES OF QUANTUM CHAOS

$$s_i = e_i - e_{i-1}$$

$$\langle \bar{r} \rangle = \frac{1}{D} \sum_{n=1}^{D} \bar{r}_n, \quad \text{where} \quad \bar{r}_n = \frac{\min(s_n, s_{n-1})}{\max(s_n, s_{n-1})}$$

$$\eta = \frac{\langle \bar{r} \rangle - \langle \bar{r} \rangle_P}{\langle \bar{r} \rangle_{\mathrm{GOE}} - \langle \bar{r} \rangle_P}$$

We complement this quantity with a chaotic measure based on eigenstate statistics. By expanding each eigenstate of the system $|\psi_i\rangle$ onto those of a suitable reference basis $|\phi_j\rangle$, one obtains a set of coefficients $x \equiv |c_{ij}|^2$ obeying a distribution that depends on the universality class of the system [29–31]. For the orthogonal ensemble, this distribution is

$$\mathrm{PDF}(x) = \frac{\Gamma\left(\frac{D}{2}\right)}{\Gamma\left(\frac{D-1}{2}\right)} \frac{1}{\sqrt{\pi x}} (1-x)^{\frac{D-3}{2}}, \qquad (19)$$

where D is the dimension of the system and $\Gamma(z)$ is the Gamma function. We then define a measure of chaoticity using the Kolmogorov-Smirnov statistic [33], which compares the empirical CDF of the coefficient distribution to the CDF corresponding to the orthogonal ensemble distribution (19):

$$\Delta_{\mathrm{KS}} = 1 - \sup_x |\mathrm{eCDF}(x) - \mathrm{CDF}(x)|, \qquad (20)$$

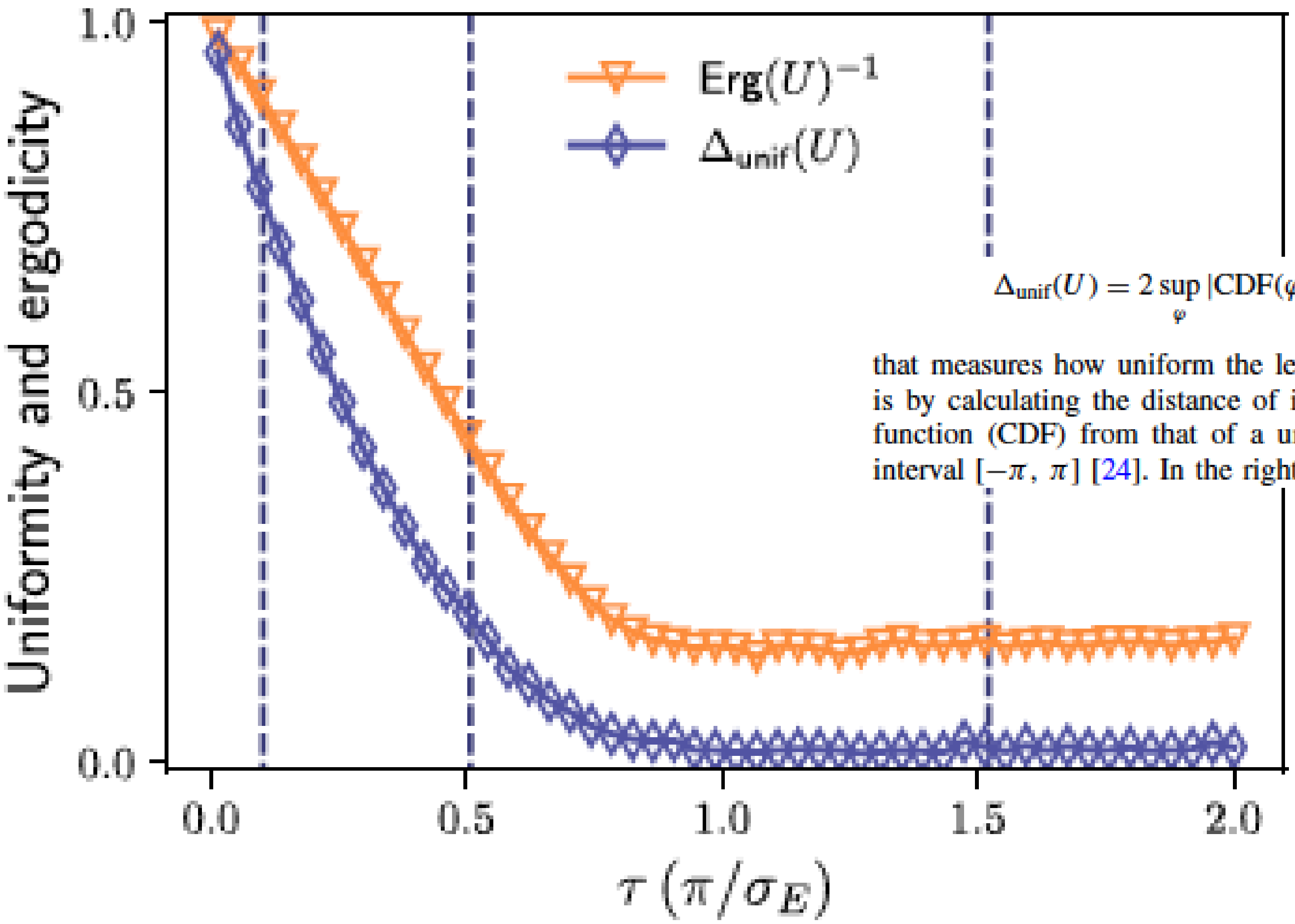
such that $\Delta_{\mathrm{KS}} \approx 1$ for a chaotic system, and it decreases for integrable systems.

Modelo RMT

$$H_{\mathrm{RMT}} = \frac{H_0 + kV}{\sqrt{1+k^2}}$$

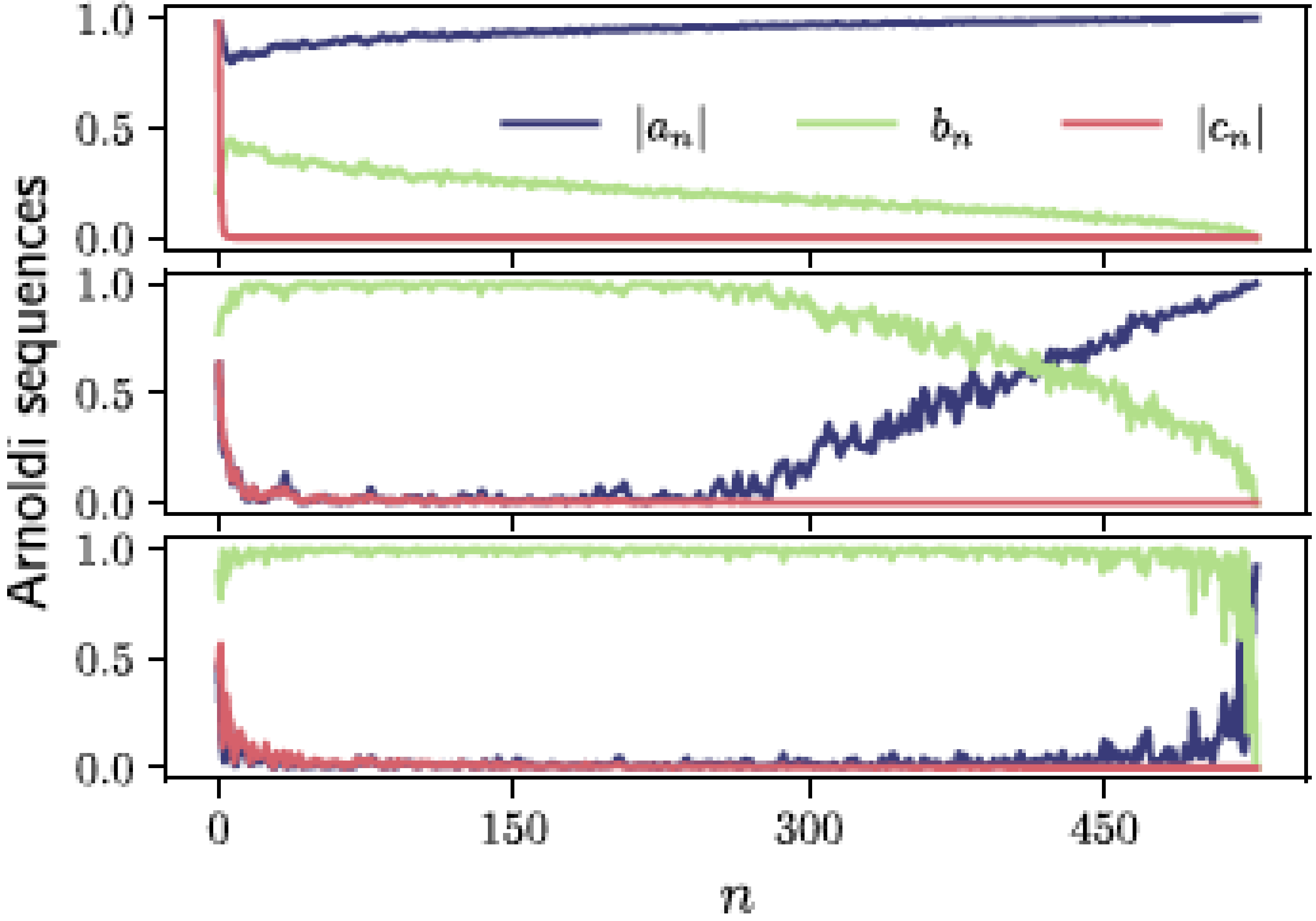
with H_0 a diagonal matrix with its nonzero elements chosen as real Gaussian variables with unit standard deviation, describing the integrable part; on the other hand, V is taken to be a real-valued banded random matrix of bandwidth $2b$ (such that it is a full matrix for $b = D$, the system dimension) whose values are Gaussian variables with standard deviation equal to $1/\sqrt{b+1}$, such that its spectral variance is of order unity for large enough b. In the spirit of Ref. [41], we define a transition parameter for this model as $\Lambda = k^2 D^2 / 2\pi(b+1)$, which makes the η transition from Poissonian to GOE statistics dimension-independent; see Appendix C.

$$\Lambda = k^2 D^2 / 2\pi(b+1)$$

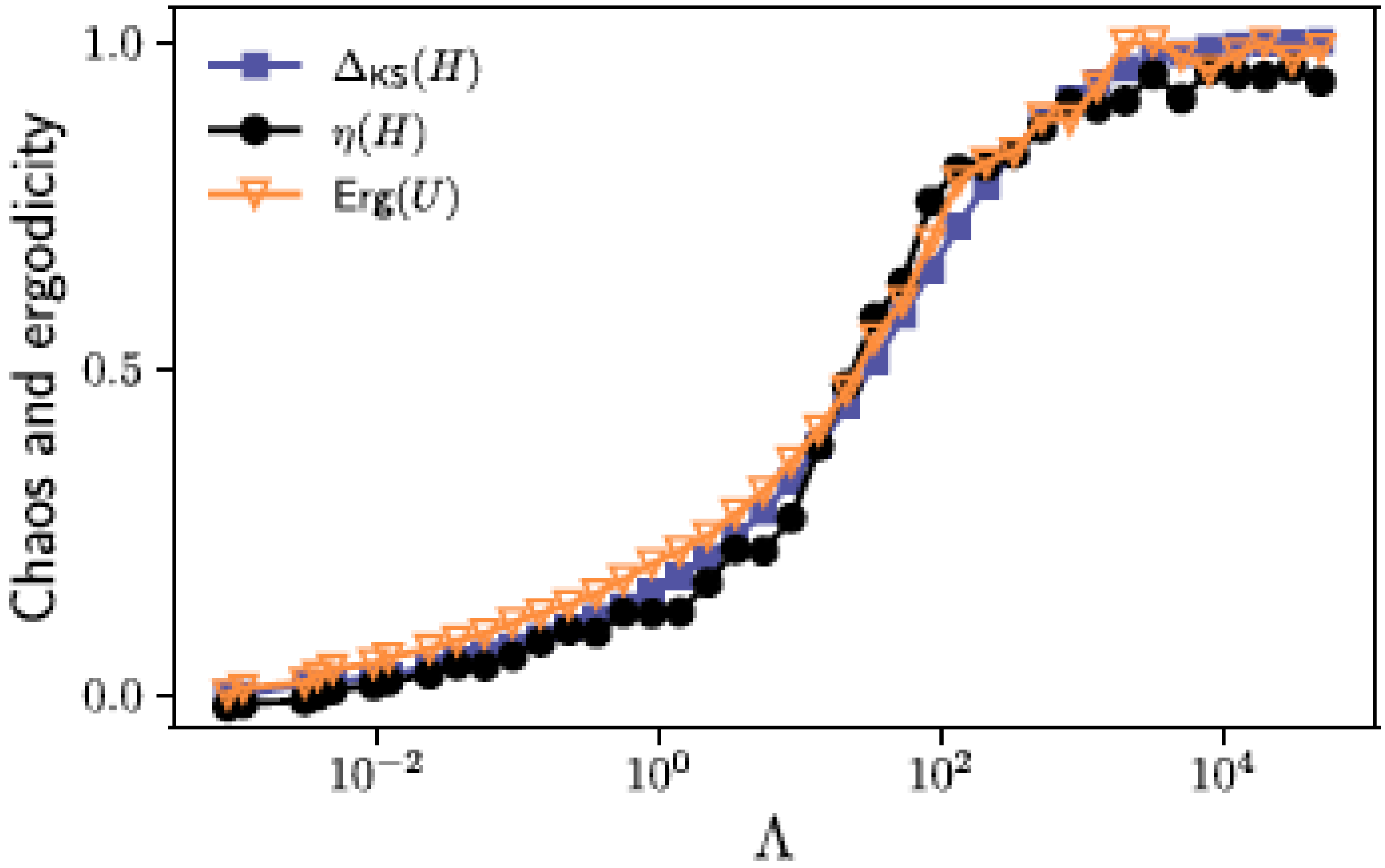


$$\Delta_{\mathrm{unif}}(U) = 2 \sup_{\varphi} |\mathrm{CDF}(\varphi) - \mathrm{CDF}_{\mathrm{unif}}(\varphi)| \tag{16}$$

that measures how uniform the level density of the unitary is by calculating the distance of its cumulative distribution function (CDF) from that of a uniform distribution in the interval $[-\pi, \pi]$ [24]. In the right panel of Fig. 1 we show



Arnoldi sequences
$|a_n|$
b_n
$|c_n|$
1.0
0.5
0.0
0
150
300
450
n



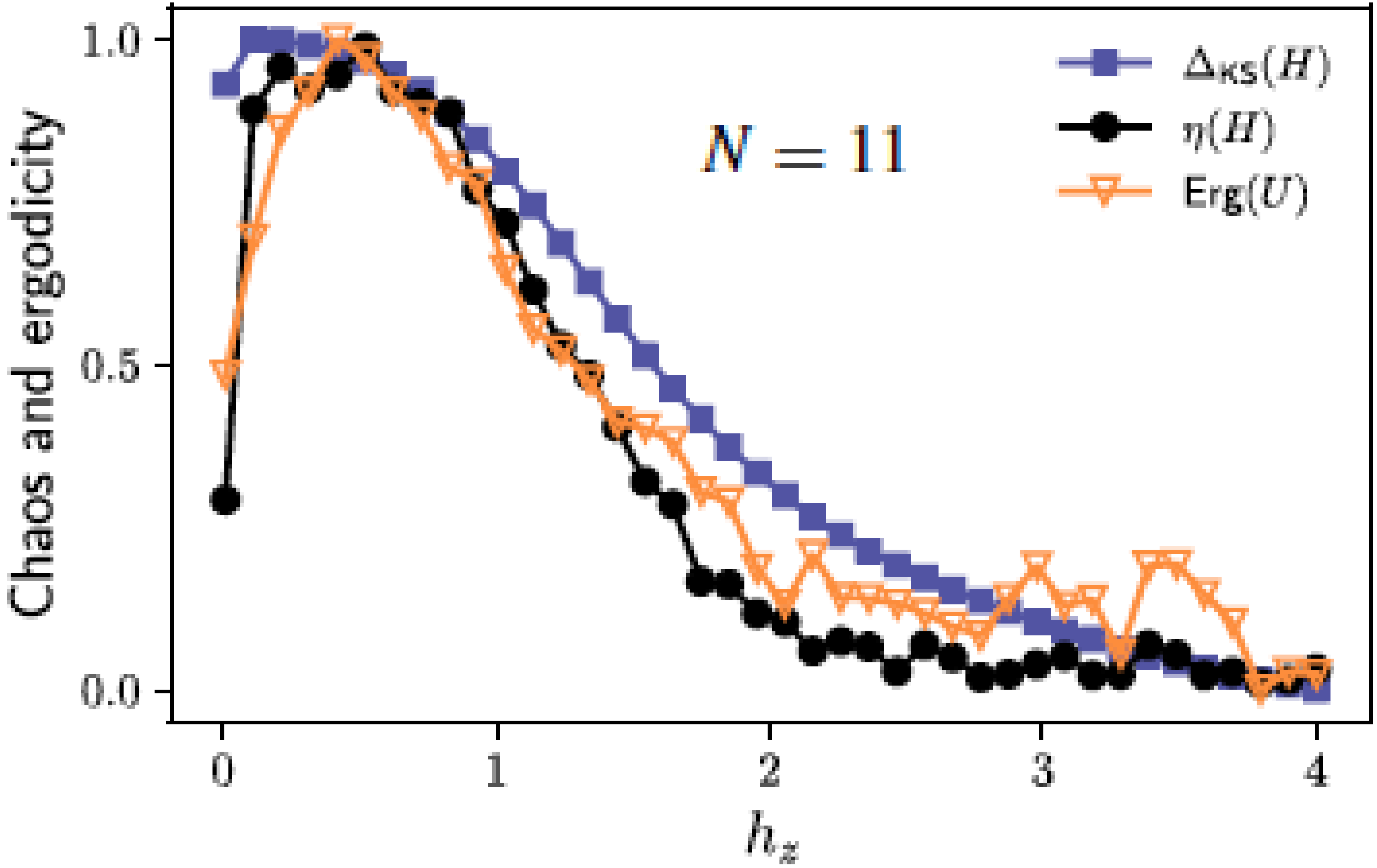
$\Delta_{KS}(H)$
$\eta(H)$
Erg(U)
Chaos and ergodicity
1.0
0.5
0.0
10^{-2}
10^{0}
10^{2}
10^{4}
Λ

The spin chain

$$H = \sum_{i=1}^{N} \left(\sigma_x^{(i)} + h_z \delta^{(i)} \sigma_z^{(i)} \right) - \sum_{i=1}^{N-1} \sigma_z^{(i)} \sigma_z^{(i+1)}$$

$$U = e^{-i\tau H}$$

$$\tau = 0.15\,(2\pi)$$



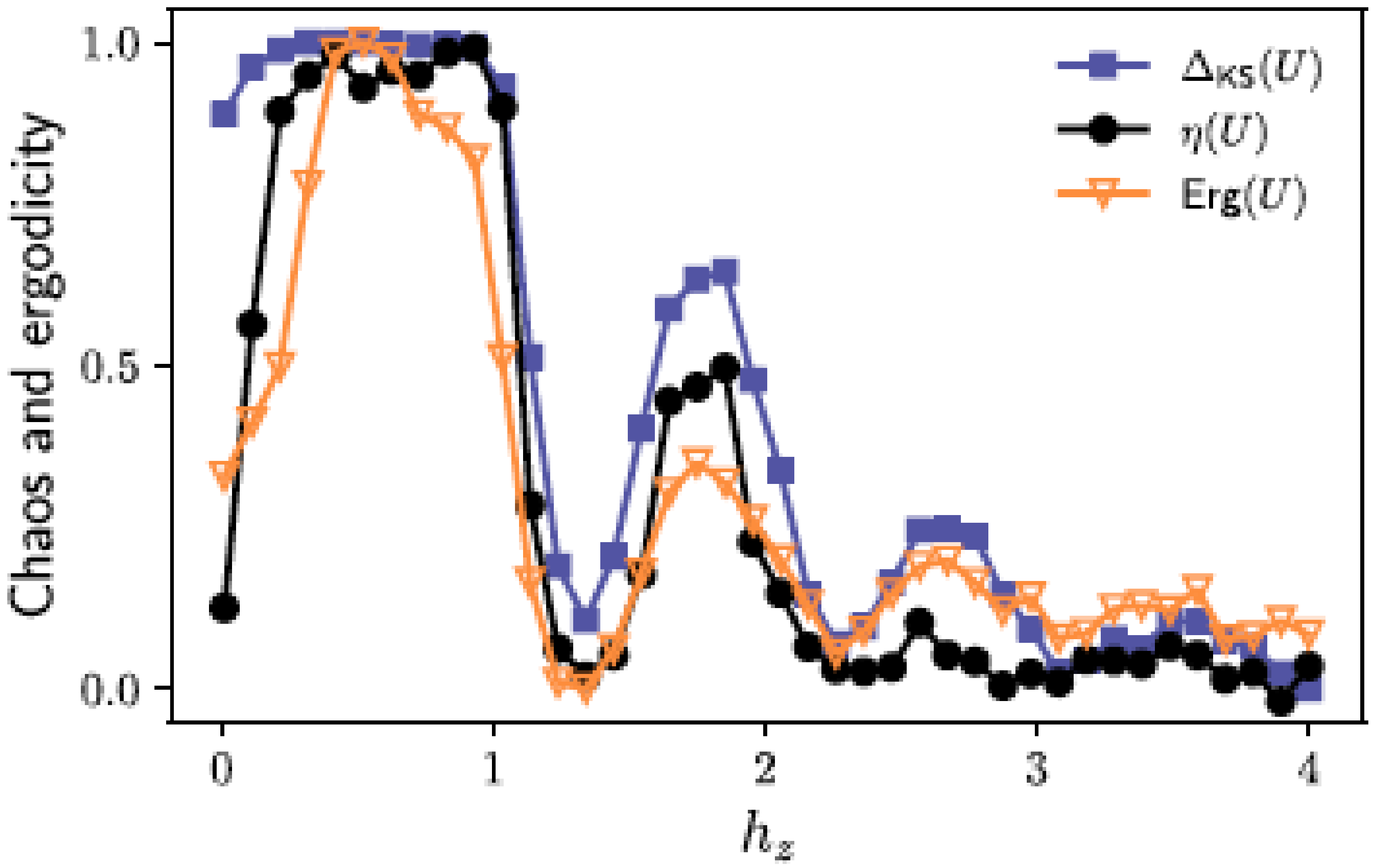
$\Delta_{KS}(H)$
$\eta(H)$
Erg(U)
$N = 11$
Chaos and ergodicity
1.0
0.5
0.0
0
1
2
3
4
h_z

The Trotterized spin chain

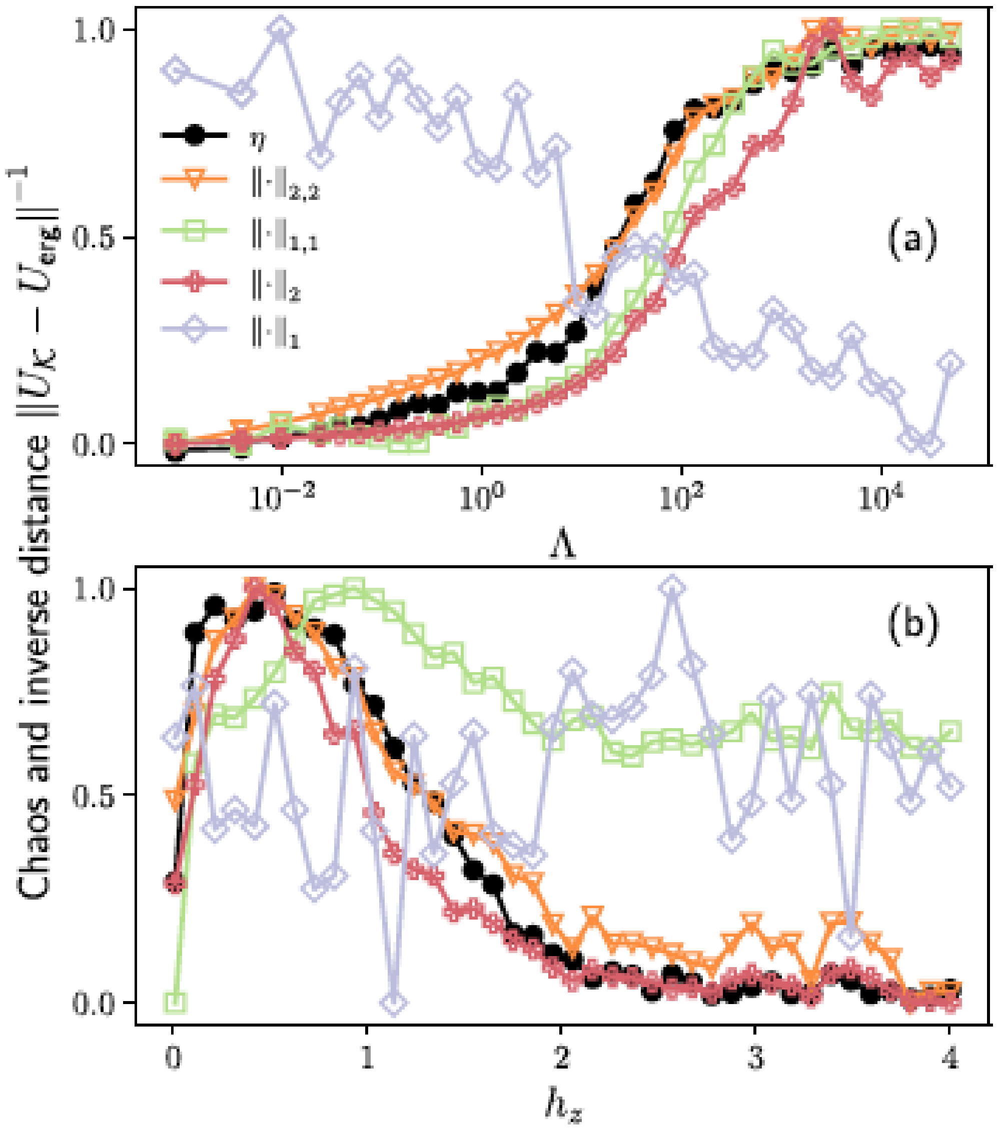
$$U = e^{-i\tau H_{zz}} e^{-i\tau H_s}, \quad \text{where} \;\; H_{zz} = -\sum_{i=1}^{N-1} \sigma_z^{(i)} \sigma_z^{(i+1)}$$

$$H_s = \sum_{i=1}^{N} \left(\sigma_x^{(i)} + h_z \delta^{(i)} \sigma_z^{(i)} \right)$$

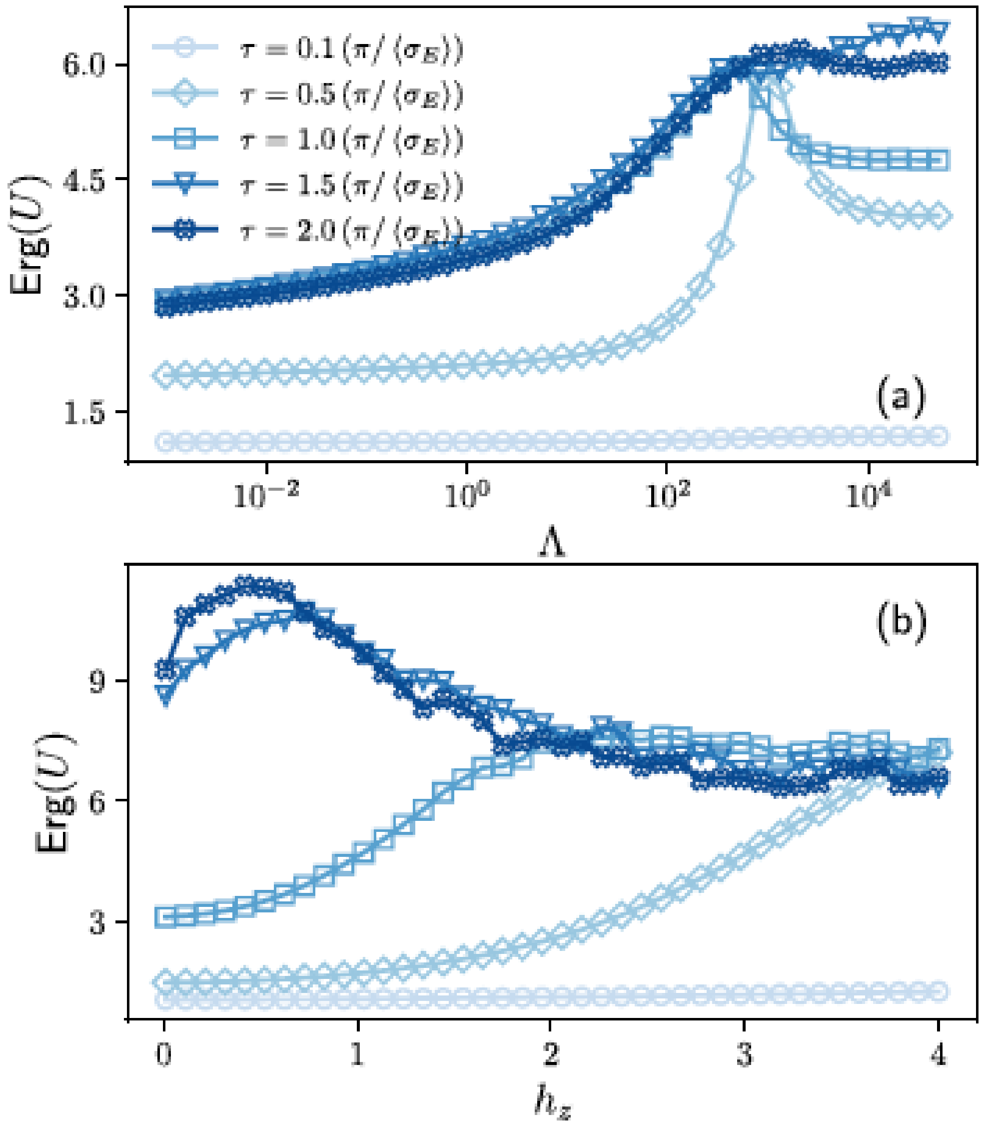
$$H(t) = H_{zz} + \tau H_s \sum_{n=-\infty}^{\infty} \delta(t - n\tau)$$



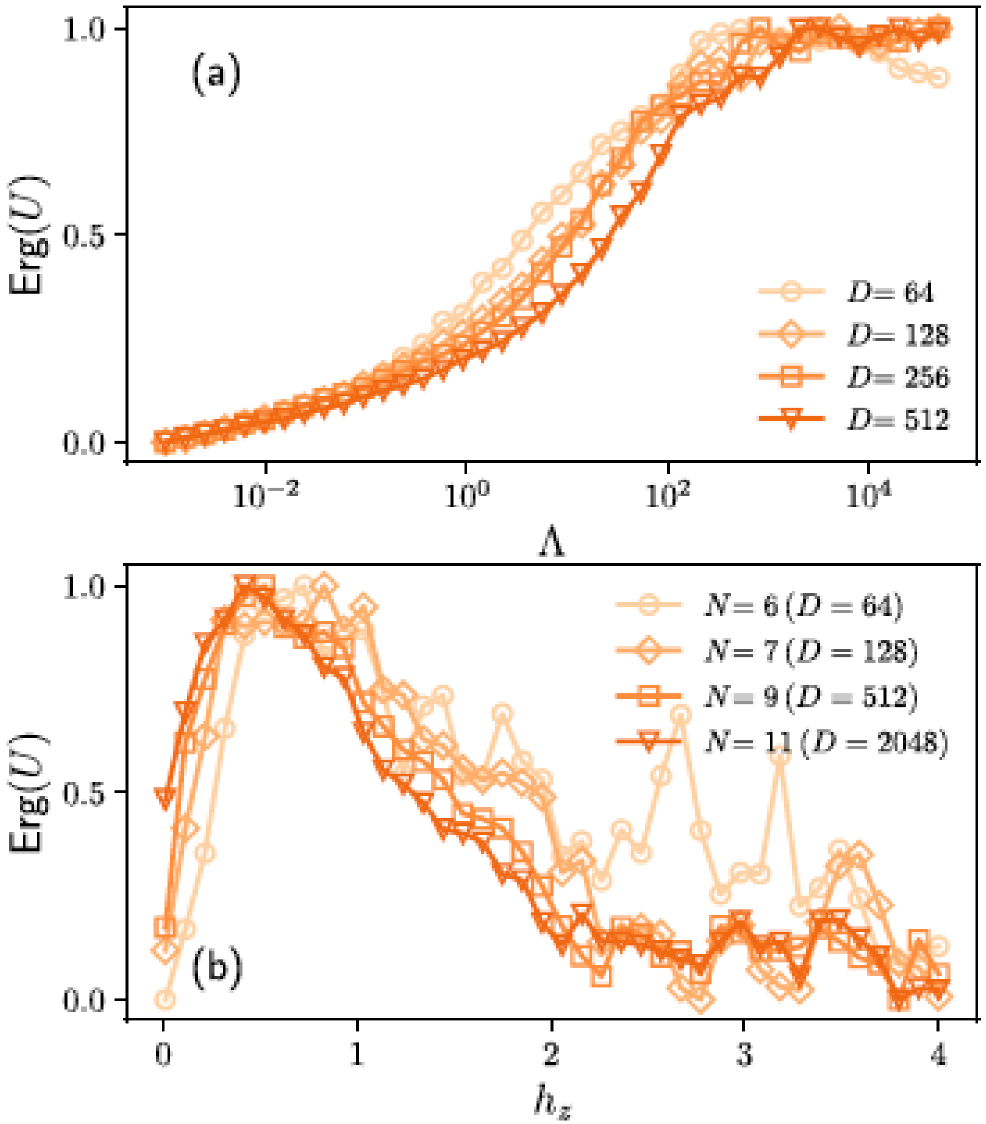
Chaos and ergodicity
1.0
0.5
0.0
0
1
2
3
4
h_z
$\Delta_{KS}(U)$
$\eta(U)$
$\mathrm{Erg}(U)$



(a)
(b)
η
‖·‖2,2
‖·‖1,1
‖·‖2
‖·‖1
Chaos and inverse distance ‖U𝒦 − Uerg‖^−1
Λ
hz



τ = 0.1 (π/⟨σ_E⟩)
τ = 0.5 (π/⟨σ_E⟩)
τ = 1.0 (π/⟨σ_E⟩)
τ = 1.5 (π/⟨σ_E⟩)
τ = 2.0 (π/⟨σ_E⟩)
Erg(U)
Λ
(a)
(b)
h_z



(a)
D= 64
D= 128
D= 256
D= 512
Erg(U)
Λ
(b)
N= 6 (D = 64)
N= 7 (D = 128)
N= 9 (D = 512)
N= 11 (D = 2048)
h_z

Exploring quantum ergodicity of unitary evolution through the Krylov approach

Gastón F. Scialchi,[1,2,*] Augusto J. Roncaglia,[1,2] Carlos Pineda,[3] and Diego A. Wisniacki[1,2,†]
[1]*Facultad de Ciencias Exactas y Naturales, Departamento de Física, Universidad de Buenos Aires, Buenos Aires 1428, Argentina*
[2]*CONICET - Instituto de Física de Buenos Aires (IFIBA), Universidad de Buenos Aires, Buenos Aires 1428, Argentina*
[3]*Instituto de Física, Universidad Nacional Autónoma de México, Ciudad de México 01000, Mexico*

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In recent years, there has been growing interest in characterizing the complexity of quantum evolutions of interacting many-body systems. When a time-independent Hamiltonian governs the dynamics, Krylov complexity has emerged as a powerful tool. For unitary evolutions like kicked systems or Trotterized dynamics, a similar formulation based on the Arnoldi approach has been proposed yielding a new notion of quantum ergodicity [P. Suchsland, R. Moessner, and P. W. Claeys, Phys. Rev. B **111**, 014309 (2025)]. In this work, we show that this formulation is robust for observing the transition from integrability to chaos in both autonomous and kicked systems. Examples from random matrix theory and spin chains are shown in this paper.

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Assessing the saturation of Krylov complexity as a measure of chaos

Bernardo L. Español and Diego A. Wisniacki
Departamento de Física "J. J. Giambiagi" and IFIBA, FCEyN, Universidad de Buenos Aires, 1428 Buenos Aires, Argentina

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Krylov complexity is a novel approach to study how an operator spreads over a specific basis. Recently, it has been stated that this quantity has a long-time saturation that depends on the amount of chaos in the system. Since this quantity not only depends on the Hamiltonian but also on the chosen operator, in this work we study the level of generality of this hypothesis by studying how the saturation value varies in the integrability to chaos transition when different operators are expanded. To do this, we work with an Ising chain with a longitudinal-transverse magnetic field and compare the saturation of the Krylov complexity with the standard spectral measure of quantum chaos. Our numerical results show that the usefulness of this quantity as a predictor of the chaoticity is strongly dependent on the chosen operator.

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Integrability-to-chaos transition through the Krylov approach for state evolution

Gastón F. Scialchi,[1,2,*] Augusto J. Roncaglia,[1,2] and Diego A. Wisniacki[1,2,†]
[1]*Universidad de Buenos Aires, Facultad de Ciencias Exactas y Naturales, Departamento de Física, Ciudad Universitaria, 1428 Buenos Aires, Argentina*
[2]*CONICET–Universidad de Buenos Aires, Instituto de Física de Buenos Aires (IFIBA), Ciudad Universitaria, 1428 Buenos Aires, Argentina*

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The complexity of quantum evolutions can be understood by examining their spread in a chosen basis. Recent research has stressed the fact that the Krylov basis is particularly adept at minimizing this spread [Balasubramanian *et al.*, Phys. Rev. D **106**, 046007 (2022)]. This property assigns a central role to the Krylov basis in the investigation of quantum chaos. Here, we delve into the transition from integrability to chaos using the Krylov approach, employing an Ising spin chain and a banded random matrix model as our testing models. Our findings indicate that both the saturation of Krylov complexity and the spread of the Lanczos coefficients can exhibit a significant dependence on the initial condition. However, both quantities can gauge dynamical quantum chaos with a proper choice of the initial state.

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Exploring quantum ergodicity of unitary evolution through the Krylov approach

Gastón F. Scialchi,[1,2,*] Augusto J. Roncaglia,[1,2] Carlos Pineda,[3] and Diego A. Wisniacki[1,2,†]
[1]*Facultad de Ciencias Exactas y Naturales, Departamento de Física, Universidad de Buenos Aires, Buenos Aires 1428, Argentina*
[2]*CONICET - Instituto de Física de Buenos Aires (IFIBA), Universidad de Buenos Aires, Buenos Aires 1428, Argentina*
[3]*Instituto de Física, Universidad Nacional Autónoma de México, Ciudad de México 01000, Mexico*

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In recent years, there has been growing interest in characterizing the complexity of quantum evolutions of interacting many-body systems. When a time-independent Hamiltonian governs the dynamics, Krylov complexity has emerged as a powerful tool. For unitary evolutions like kicked systems or Trotterized dynamics, a similar formulation based on the Arnoldi approach has been proposed yielding a new notion of quantum ergodicity [P. Suchsland, R. Moessner, and P. W. Claeys, Phys. Rev. B **111**, 014309 (2025)]. In this work, we show that this formulation is robust for observing the transition from integrability to chaos in both autonomous and kicked systems. Examples from random matrix theory and spin chains are shown in this paper.

DOI: 10.1103/PhysRevE.111.014220

Calculo de autovalores usando Krylov

Algoritmo de Arnoldi

Se quiere resolver el problema de autovalores y autovectores

$$Av = \lambda v \qquad \mathrm{A} \in \mathbb{C}^{m \times m}$$

Considerando un vector arbitrario $b \in \mathbb{C}^{m \times 1}$, se puede construir el **subespacio de Krylov**

$$\mathcal{K}_m(A, b) = gen\{b, Ab, A^2 b, \ldots, A^{m-1} b\}$$

El método iterativo de Arnoldi, permite obtener una base ortonormal de $\mathcal{K}_m(A, b)$. Los vectores de esta nueva base, permiten definir una matriz unitaria Q que transformar a la matriz A,
en una matriz de Hessenber H

$$A = QHQ^*$$

$$AQ = QH$$

Algoritmo de Arnoldi

Si en lugar de considerar los m elementos de la base, nos limitamos a solo $\boldsymbol{k} \ll \boldsymbol{m}$ de ellos, la transformación sigue siendo válida si consideramos **la sección superior izquierda de $\boldsymbol{H}$**

$$\boldsymbol{AQ_k = Q_{k+1}H_k}$$

$$A\begin{bmatrix} q_1 & \cdots & q_k \end{bmatrix} = \begin{bmatrix} q_1 & \cdots & q_k & q_{k+1} \end{bmatrix} \begin{bmatrix} h_{11} & \cdots & h_{1k} \\ h_{21} & h_{22} & \cdots \\ 0 & h_{32} & \cdots \\ \vdots & \ddots & h_{k,k} \\ 0 & 0\cdots & h_{k+1,k} \end{bmatrix}.$$

Los que nos da la relación de recurrencia,

$$Aq_k = h_{1,k}q_1 + \cdots + h_{k,k}q_k + h_{k+1,k}q_{k+1}$$

Algoritmo de Arnoldi

De esto último, podemos calcular los elementos de las matrices

$$q_{k+1} = \frac{Aq_k - \sum_j h_{j,k} q_j}{\left\| Aq_k - \sum_j h_{j,k} q_j \right\|}$$

$$h_{j,k} = q_j^* A q_k$$

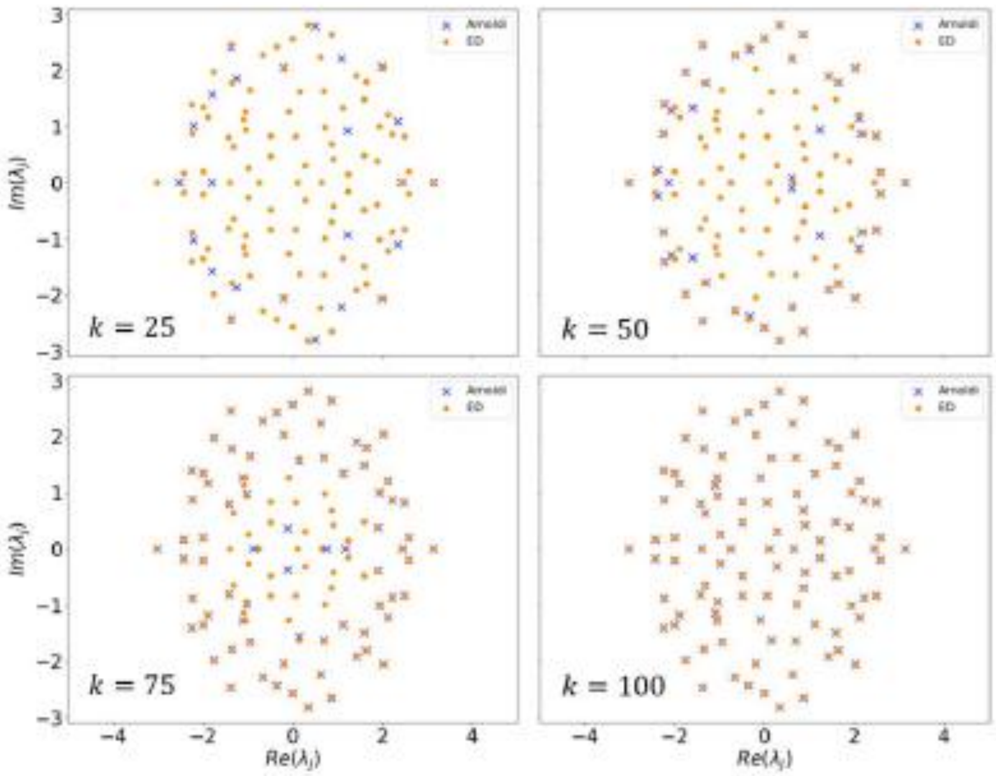
$$h_{k+1,k} = \left\| Aq_k - \sum_j h_{j,k} q_j \right\|$$

- ❑ Los autovalores de la matriz H, conocidos como **autovalores de Ritz**, son una buena aproximación de los autovalores de la matriz original A.

Algoritmo de Arnoldi

En la figura, un ejemplo con una matriz

$$A \in \mathbb{C}^{100\times100}$$



Arnoldi desplazado e invertido

Shift

$$(A - \sigma I)^{-1} u = \theta u$$

$(A - \sigma I)^{-1} u = \theta u$ **es equivalente a** $Av = \lambda v$

$$\theta = \frac{1}{\lambda - \sigma}$$

Entonces, para hallar un vector de la base ortonormal, debemos resolver

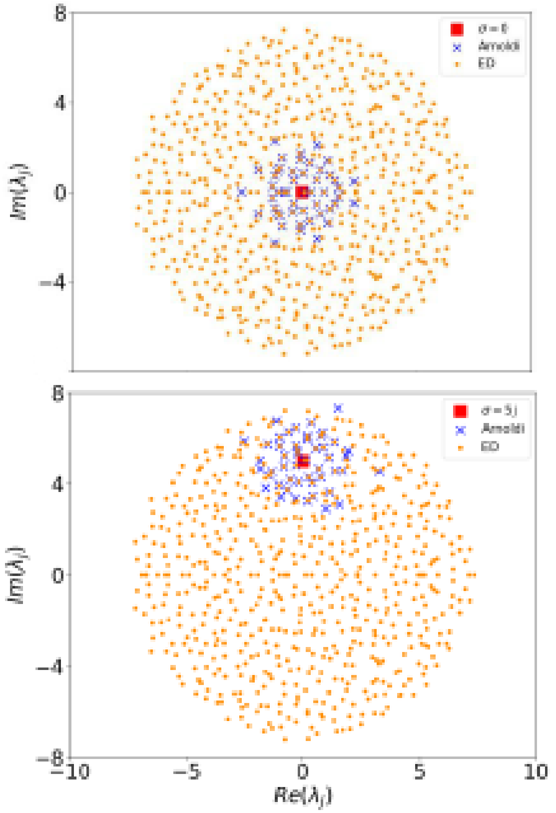
$$u_{k+1} = (A - \sigma I)^{-1} q_k$$

$$(A - \sigma I) u_{k+1} = q_k$$

Arnoldi desplazado e invertido

En la figuras, un ejemplo con una matriz arbitraria
$A \in \mathbb{C}^{625\times 625}$, utilizando $k = 50$

- En ambos ejemplos, el algoritmo tiende a calcular los autovalores **cercanos** al shift σ.



Control and quantum chaos @dfuba

Lionel Martinez

Tomas Busto

Gastón Scialchi

DAW

Old members related with the presented work

Nicolas Mirkin

Martin Larocca

Emiliano Fortes

Bernardo Español

Tomás Nottenson